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[Continued on next page]

(54) Title: METHODS FOR INHIBITING FASCIN

(57) Abstract: The invention relates to compositions and methods useful for inhibiting fascin. These compositions and methods can be used to inhibit fascin-related diseases. For example, according to the invention inhibition of fascin inhibits metastasis of tumor cells in mammals.

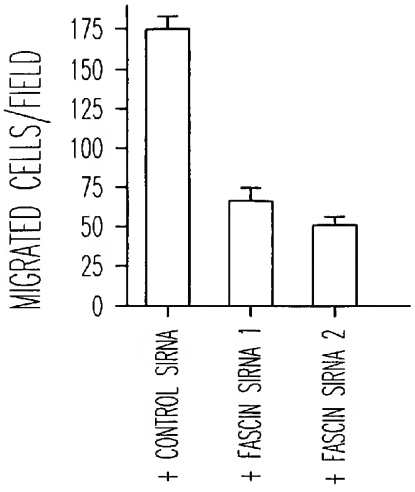

Fig. 7B

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PCT PATENT APPLICATION

METHODS FOR INHIBITING FASCIN

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METHODS FOR INHIBITING FASCIN

Government Funding

The invention described in this application was made with funds from Department of Defense Grant Number BC050558. The United States government has certain rights in the invention.

Related Applications

This application claims priority to the filing date of U.S. Provisional Application Ser. No. 60/989,609, filed November 21, 2007, the contents of which are specifically incorporated by reference herein in their entirety.

This application is also related to U.S. Application Ser. No. 10/551152 filed March 26, 2004, U.S. Application Ser. No. 10/551158 filed March 26, 2004, PCT Application Ser. No. PCT/US04/09380 filed March 26, 2004, U.S. Provisional Application Nos.: 60/458,827, filed March 28, 2003. The entire contents of each of the above-referenced applications are hereby specifically incorporated herein by reference in their entireties.

Field of the Invention

The invention relates to novel compositions and methods for inhibiting fascin expression and/or activity. According to the invention, such inhibition of fascin leads to inhibition of cell migration, including metastasis of cancer cells. The invention also relates to methods for identifying agents that modulate the expression and/or activity of fascin.

Background of the Invention

Despite the significant improvement in both diagnostic and therapeutic modalities for the treatment of cancer patients, tumor metastasis is still the major cause of mortality in cancer. Metastasis is the multi-step process wherein a primary tumor spreads from its initial site to secondary tissues/organs. This metastatic

process is selective for cells that succeed in cell migration/invasion, embolization, survival in the circulation, arrest in a distant capillary bed, and extravasation into and multiplication within the organ parenchyma. Since tumor spreading is responsible for the majority of deaths of cancer patients, development of therapeutic agents that inhibit tumor metastasis is very desirable.

Summary of the Invention

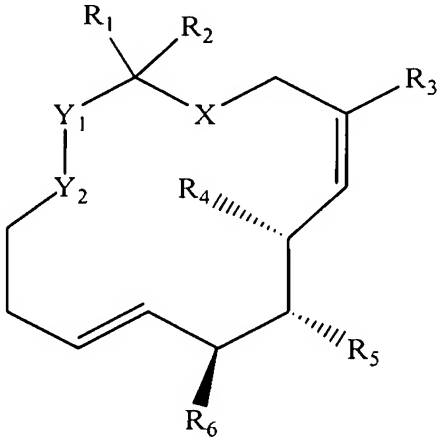
The invention relates to methods of inhibiting fascin expression and/or activity. Fascin bundles F-actin polymers into highly dynamic membrane protrusions in motile cells. These actin-based, crosslinked protrusions support the outward extension of the leading edge of cellular mobility. As illustrated herein, knockdown of fascin expression in highly invasive breast tumor cells inhibits cell migration and invasion both *in vitro* and within *in vivo* animal models of metastatic cancer. The invention provides agents that modulate fascin expression and/or activity. Such agents are useful for treating and inhibiting diseases and conditions associated with fascin expression and/or activity, including metastatic cancer.

Therefore, one aspect of the invention is a method of inhibiting fascin expression and/or activity, comprising administering an effective amount of a fascin inhibitor to a cell expressing fascin to thereby inhibit the fascin expression or activity in the cell. For example, the fascin inhibitor can be an inhibitory nucleic acid that binds specifically to a fascin RNA or DNA consisting of SEQ ID NO:2, 4, 6 or 8, a small molecule, a fascin polypeptide fragment, or an antibody that binds specifically to fascin.

In some embodiments, the fascin inhibitor is an inhibitory nucleic acid that binds specifically to a fascin RNA or DNA consisting of SEQ ID NO:2, 4, 6 or 8. The inhibitory nucleic acid can be an RNA or DNA, having a sequence that can be any of SEQ ID NOs:13-62, or a combination thereof. For example, the inhibitory nucleic acid can be administered by administering an expression vector that includes an expression cassette capable of directing the expression of the inhibitory nucleic acid.

The fascin inhibitor can also be an anti-fascin antibody. For example, the antibody can block actin binding to a fascin actin-binding site or can bind specifically to a fascin actin-binding site. In some embodiments, the fascin actin-binding site includes any of fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250. In other embodiments, the fascin actin-binding site includes any of fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473. For example, the antibody can block actin binding to one or both of fascin amino acids His392 and His474 when bound to fascin protein. In other embodiments, the antibody can bind to one or both of fascin amino acids His392 and His474 when bound to fascin protein.

In some embodiments, the fascin inhibitor is a compound of formula I:



wherein:

X is CH, N, NH or O;

R_1 is OH, CZ_3 or R_1 and R_2 together are –C=O, wherein Z is halo;

R_2 is OH, CZ_3 or R_1 and R_2 together are –C=O, wherein Z is halo;

R_3 is H or lower alkyl;

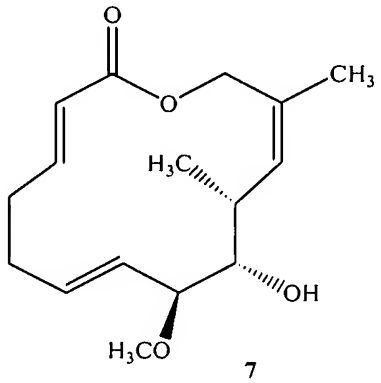
R_4 is H or lower alkyl;

R_5 is OH;

R_6 is alkyloxy;

Y_1 and Y_2 are separately $-CH_2-$ or Y_1 and Y_2 together form $-C=C-$

or a pharmaceutically acceptable salt thereof. Examples of compounds that can be used include any one of the following compounds, or a combination of such compounds:



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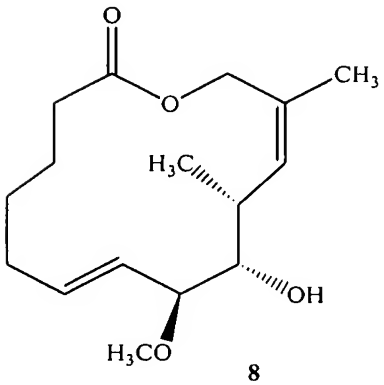

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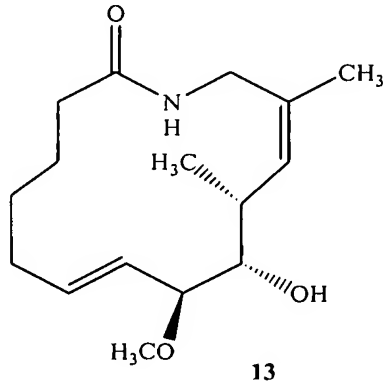

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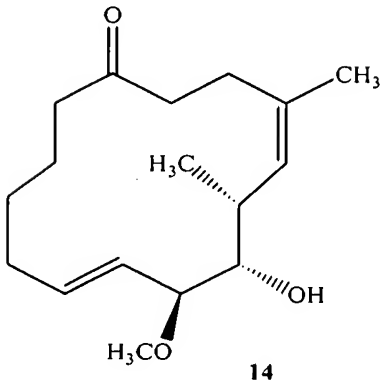

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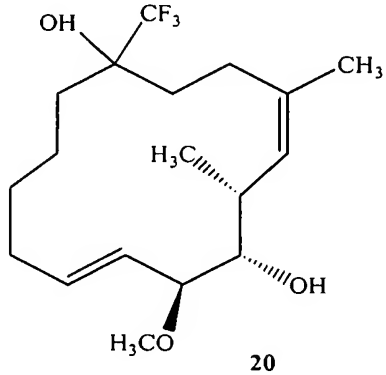

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In some embodiments, the fascin inhibitor is not a migrastatin analog of formula I and is not compound 7, 8, 13, 14 or 20.

The cell is in an animal, for example, a human. Such an animal or human can be suffering from a disease or condition, for example, a disease involving expression or over-expression of fascin. The disease or condition can, for example, be a metastatic cancer, a neuronal disorder, neuronal degeneration, an inflammatory condition, a viral infection, a bacterial infection, lymphoid hyperplasia, Hodgkin's disease or ischemia-related tissue damage. In some embodiments, the cancer is a carcinoma, lymphoma, sarcoma, melanoma, astrocytoma, mesothelioma cells, ovarian carcinoma, colon carcinoma, pancreatic carcinoma, esophageal carcinoma, stomach carcinoma, lung carcinoma, urinary carcinoma, bladder carcinoma, breast cancer, gastric cancer, leukemia, lung cancer, colon cancer, central nervous system cancer, melanoma, ovarian cancer, renal cancer or prostate cancer.

Another aspect of the invention is a method of identifying an inhibitor of fascin, comprising: (a) contacting at least one protein or peptide having a fascin sequence with at least one test agent for a sufficient time to allow the components to interact; and (b) determining whether binding between the at least one protein or peptide having a fascin sequence and the test agent has occurred, wherein binding between the at least one protein or peptide having a fascin sequence and test agent is indicative that the test agent is an inhibitor of cancer metastasis. For example, the test agent can block actin binding to a fascin actin-binding site or binds to a fascin actin-binding site. The fascin actin-binding site can include fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250. In other embodiments, the fascin actin-binding site can include fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473. For example, the test agent can block actin binding to one or both of fascin amino acids His392 and His474 when bound to fascin protein. In other embodiments, the test agent binds to one or both of fascin amino acids

His392 and His474 when bound to fascin protein. The method can further include determining the binding constant of the test agent for fascin. The method can also determining whether the test agent inhibits fascin-mediated actin bundle formation. For example, the actin employed can be F-actin.

Another aspect of the invention is a method for identifying an inhibitor of fascin, comprising: (a) generating a three-dimensional structural image of a fascin binding site from fascin atomic coordinates for fascin amino acids Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250, according to Table 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms; and (b) designing or selecting a potential inhibitor to reside within the fascin binding site to thereby identify an inhibitor of fascin.

Another aspect of the invention is a method for identifying an inhibitor of fascin, comprising: (a) generating a three-dimensional structural image of a fascin binding site from fascin atomic coordinates for fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473 according to Table 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms; and (b) designing or selecting a potential inhibitor to reside within the fascin binding site to thereby identify an inhibitor of fascin.

Such methods can further include synthesizing or obtaining the potential inhibitor, contacting the potential inhibitor with fascin, and ascertaining whether the potential inhibitor binds to fascin. In some embodiments, the potential inhibitor is no larger than about eight (8) angstroms by about ten (10) angstroms by about ten (10) angstroms.

In some embodiments the method is performed using a computer system comprising the fascin atomic coordinates as a data set. The inhibitor of fascin that is identified can be an inhibitor of metastatic cancer.

Another aspect of the invention is a machine readable storage medium, comprising fascin atomic coordinates of Table 2. In some embodiments, the machine readable storage medium includes fascin atomic coordinates for fascin amino acids Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250, according to Table 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms. In other embodiments, the machine readable storage medium includes fascin atomic coordinates for fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473 according to Table 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms. Alternatively, the machine readable storage medium can include the atomic coordinates for both fascin actin sites.

Another aspect of the invention is a fascin inhibitor comprising an inhibitory nucleic acid that binds specifically to a fascin RNA or DNA consisting of SEQ ID NO:2, 4, 6 or 8, a small molecule, a fascin polypeptide fragment, or an antibody that binds specifically to fascin. For example, the inhibitory nucleic acid can be an RNA or DNA consisting of any of SEQ ID NOs:13-62. In some embodiments, the inhibitory nucleic acid is expressed in an expression vector comprising an expression cassette that directs the expression of a fascin inhibitory nucleic acid. The antibody can, for example, bind specifically to a fascin actin-binding site, or blocks actin-binding to a fascin actin-binding site, wherein the actin-binding site comprises fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250. In other embodiments, the antibody can bind specifically to a fascin actin-binding site, or blocks actin-binding to a fascin actin-binding site, wherein the actin-binding site comprises fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473. For example, the antibody can be generated using a polypeptide with a

sequence that includes fascin amino acids 259 through 493. Alternatively, for example, the antibody can be generated using a polypeptide with SEQ ID NO:9, 10 and/or 12. The fascin polypeptide fragment that is a fascin inhibit can include a peptide with fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250. Alternatively, for example, the fascin polypeptide fragment that is a fascin inhibitor can include fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473. Thus, according to the invention, the fascin polypeptide fragment can consist of fascin amino acids 259 through 493, or a fascin polypeptide with SEQ ID NO:9, 10 and/or 12

Another aspect of the invention is a method of treating or inhibiting metastatic cancer in a patient, comprising administering to the patient, a fascin inhibitor of the invention.

Another aspect of the invention involves use of a fascin inhibitor in the manufacture of a medicament. For example, the medicament can be used for the treatment of metastatic cancer, a neuronal disorder, neuronal degeneration, an inflammatory condition, a viral infection, a bacterial infection, lymphoid hyperplasia, Hodgkin's disease or ischemia-related tissue damage. In some embodiments, the medicament is used for the treatment or inhibition of metastatic cancer or cancer cell in a mammal.

Brief Description of the Figures

FIG. 1. Inhibition of mouse breast tumor 4T1 cell migration by core macroketone and core macrolactam. (A) Chemical structures of migrastatin, core macroketone, and core macrolactam. (B) Wound-healing assay showed that core macroketone (2 μM) and macrolactam (2 μM) inhibited the migration of mouse breast tumor 4T1 cells induced by serum. (C) Chamber assay of the effect of various concentrations of core macroketone on serum-induced 4T1 cell migration.

(D) Chamber assay of the effect of core macrolactam on the serum-induced migration of 4T1 cells. Data represent mean ± SD of three experiments.

FIG. 2. Inhibition of human tumor cell migration by core macroketone and core macrolactam. (A) Wound-healing assay showed that core macroketone (20 μM) and macrolactam (20 μM) inhibited the migration of human breast tumor MDA-MB-231 cells induced by serum. (B) IC_{50} of core macroketone and core macrolactam on serum-induced migrations of human breast, colon, and prostate tumor cells. (C) Wound-healing assay showed that core macroketone (200 μM) and macrolactam (200 μM) had no effect on the migration of mouse embryonic fibroblast (MEF) cells induced by serum. (D) IC_{50} of core macroketone and core macrolactam on serum (10% FBS)-induced migration of MEF and human mammary-gland epithelial MCF-10A cells and on N-formyl-peptide-induced (100 nM) migration of primary mouse leukocytes (neutrophils). Data are representative of three experiments.

FIG. 3. Inhibition of breast tumor metastasis by core macroketone and core macrolactam in a mouse model. (A) Lung metastasis was measured by the 6-thioguanine clonogenic assay. (B) Chemical structures of macrolactone and migrastatin semicore. (C) On the day the mice were killed, tumor diameter (in mm) was measured with an electronic caliper. Results are mean ± SD ($n = 5$). *, $P < 0.01$.

FIG. 4. Identification of fascin as the macroketone binding protein. (A) Diagram of the structure of the biotin-conjugated macroketone core. (B) Coomassie staining of affinity purified proteins. Whole cell lysates from 200 plates (10 cm) of 4T1 cells were pre-cleared with Streptavidin beads. Half of the pre-cleared lysates were incubated with biotin-conjugated macroketone (lane 1); the other half with biotin (lane 2). After addition of Streptavidin beads, the solutions were transferred to Poly-Prep chromatography columns. After extensive washes, the bound proteins were eluted and analyzed on 10% SDS-PAGE. The arrow indicates the band identified as mouse fascin 1. Molecular mass markers are indicated on the left.

FIG. 5. Binding of purified fascin to macroketone. (A) Coomassie staining of purified GST-fascin (lane 2) and GST (lane 1) proteins. (B) Neutroavidin beads were mixed with biotin or biotin-macroketone. After wash, GST or GST-fascin was

added. The reaction was incubated for 1 hour at room temperature. After wash with 300 mM NaCl, the samples were analyzed with SDS-PAGE. Lanes 5 and 6 were loaded with GST or GST-fascin proteins as controls. The top panel was probed with anti-GST antibody. The same filter was re-probed with anti-fascin antibody (the bottom panel). (C) Competition of unlabeled macroketone with biotin-conjugated macroketone to fascin. Increasing amounts of unlabeled macroketone (molar ratio of 1:1 and 10:1 of unlabeled macroketone over biotin-conjugated macroketone) decreased the binding of biotin-conjugated macroketone to fascin. Data are representative of three to five similar experiments.

FIG. 6. Macroketone inhibits the actin-bundling activity of fascin. (A) Assay of the actin-bundling activity by the low-speed co-sedimentation assay. Polymerized F-actin (1 mM) was incubated with 0.125 μM or 0.25 μM purified fascin in the presence or absence of macroketone. Supernatants (S) or pellets (P) were analyzed by SDS-PAGE followed by Coomassie blue staining. A representative of five experiments with similar outcomes was shown. (B) Fluorescence microscopy of F-actin bundling. F-actin (1 mM) was incubated with fascin (0.125 μM) in the presence or absence of macroketone. Rhodamine-phalloidin was added to label actin filaments. Samples were mounted and imaged with a fluorescence microscopy. Left panel: in the absence of fascin, purified monomeric G-actin polymerized into F-actin, but without bundles. Middle panel: addition of purified fascin led to the bundling of actin polymers into thick filaments. Right panel: preincubation of fascin with macroketone decreased the ability of fascin to bundle actin polymers, thus leading to reduction of numbers of thick filaments. A representative of five experiments is shown. (C) Quantification of fluorescence microscopy-based F-actin bundling assays. Results are mean ± SD ($n=5$, •, $p<0.05$). (D) Electron microscopy of fascin-induced F-actin bundles in the presence or absence of macroketone. F-actin (1 mM) was incubated with fascin (0.125 μM) in the presence or absence of macroketone. Electron micrographs were obtained by negative staining of F-actin bundles. Representative images were shown. (E) Fascin and actin interaction assay. High-speed centrifugation was used to pellet F-actin polymers. Under these conditions, fascin alone was not precipitated

and fascin could only be pulled-down by binding to F-actin polymers. While similar amounts of F-actin polymers were in the pellets in the absence and presence of macroketone (since the same amounts of F-actin polymers were added), significantly less fascin was pulled down by F-actin in the presence of macroketone

FIG. 7. Role of fascin in tumor cell migration. (A) Western blots showing that fascin siRNAs decreased the expression of fascin proteins. (B) Boyden chamber migration assay with 4T1 cells treated with control siRNA and two fascin siRNAs. Fascin siRNA treatment impaired the serum-induced migration of 4T1 cells. Results are mean ± SD (n=5, $p<0.05$). (C) Boyden chamber migration assay of mouse fascin siRNA 2-treated 4T1 cells transfected with human wild-type GFP-fascin in the presence or absence of macroketone. Results are mean ± SD (n=5, $p<0.05$). (D) Western blots show the expression levels of fascin protein in whole cell extracts prepared from 4T1 cells treated with control siRNA, fascin siRNA 2, or cells transfected with both mouse fascin siRNA 2 and human wild-type GFP-fascin. (E) Western blots show the expression of fascin protein in whole cell extracts prepared from human MDA-MB-231 cells treated with control siRNA and two different fascin siRNAs. (F) Boyden chamber migration assay with MDA-MB-231 cells treated with control siRNA and two fascin siRNAs. Fascin siRNA treatment impaired the serum-induced migration of MDA-MB-231 cells. Results are mean ± SD (n=5, $p<0.05$). (G) Western blots show the expression of fascin protein in whole cell extracts prepared from non-invasive MCF-10A and metastatic MDA-MB-231 cells. (H) Chamber cell migration assay of MCF-10A cells transfected with control vector or GFP-fascin. Bottom panel shows the over-expression of fascin in MCF-10A cells. Results are mean ± SD (n=5, $p<0.05$). (I) Chamber cell migration assay of mouse fascin siRNA 2-treated 4T1 cells transected with various mutants of GFP-human fascin (h-fascin) in the presence or absence of macroketone. Bottom panel shows the over-expression of various fascin mutants in mouse fascin siRNA 2-treated 4T1 cells. Results are mean ± SD (n=5, $p<0.05$).

FIG. 8. Role of fascin in tumor metastasis. (A) In vitro Matrigel invasion assay with 4T1 cells treated with control siRNA and two different fascin siRNAs. Fascin siRNA treatment impaired serum-induced invasion of 4T1 cells. Results are

mean ± SD (n=5, $p<0.05$). (B) Primary mammary tumor growth of 4T1 cells expressing control siRNA and two fascin siRNAs. Results are mean ± SD. (C) Primary mammary tumor weight four weeks after injecting 4T1 cells expressing control siRNA and two fascin siRNAs. (D) Total number of metastatic colonies in lungs of individual mice four weeks after injecting 4T1 cells expressing control siRNA and two fascin siRNAs. (E) Representative noninvasive bioluminescence images of mice at the indicated dates after injecting human MDA-MB-231 cells expressing control siRNA and two fascin siRNAs. (F) Normalized photon flux of noninvasive bioluminescence images of mice at the indicated dates after injecting human MDA-MB-231 cells expressing control siRNA and two fascin siRNAs. Results are mean ± SD. (G) Histological analyses of the tumor tissues. Left panels, representative H&E staining of lungs from (E). Right panels, representative GFP imaging of lungs from (E). (H) Normalized photon flux of noninvasive bioluminescence images of mice at the indicated dates after injecting human MDA-MB-231 cells in the presence or absence of macroketone. Results are mean ± SD.

FIG. 9. Elevated expression of fascin in human breast cancer patients. (A) Relative expression levels of fascin mRNA in normal and breast tumor samples. (B) Relative expression levels of fascin mRNA in normal breast tissue samples, Estrogen Receptor (ER)-positive breast tumors and ER-negative breast tumors. (C) Relative expression levels of fascin mRNA in normal breast tissue samples, Progesterone Receptor (PR)-positive breast tumors and PR-negative breast tumors. (D) Representative images of fascin immunohistological staining of ER-positive and ER-negative breast tumor samples. (E) Kaplan-Meier analysis of the probability of overall survival of patients with high fascin expression (log10> 0.1) or low fascin expression. (F) Kaplan-Meier analysis of the probability of metastasis-free survival of patients with high fascin expression (log10> 0.1) or low fascin expression. (G) Relative expression levels of fascin mRNA in the Rosetta microarray data set of ER-positive and ER-negative breast cancer samples. (H) Relative expression levels of fascin mRNA in the Rosetta microarray data set of PR-positive and PR-negative breast cancer samples.

FIG. 10. Overall structures of fascin and of the complex of fascin and macroketone. (A) Left panel, structure of fascin in the absence of macroketone shown as ribbon diagram, viewed from the N- and C- terminal plane. The four β-trefoil domains are colored red, yellow, green and blue. (B) Right panel, the structure in left panel turned 90° clockwise along the y-axis. (C) Overall structure of the complex of fascin and macroketone, with macroketone binding to the surface of trefoil-1.

FIG. 11. Macroketone binding site on fascin. (A) F_{obs}-F_{calc} map contoured at 3σ showing the macroketone binding site on fascin. (B) Molecular interactions between fascin residues and macroketone. (C) Superimposition of the α-carbon of fascin molecules in the absence (red) and the presence (black) of macroketone. (D) Local conformational changes induced by macroketone binding. The structure of fascin in the absence of macroketone is shown in gray. In the original, the structure of fascin with macroketone is shown in green, red and blue. Similarly, in the original, the structure of macroketone is shown in cyan and red.

FIG. 12. Actin binding sites on fascin. (A, B) Mutagenesis studies showed that both the N- and C-termini of fascin contribute to actin binding. (C) Residues from 29 to 42 are similar in sequences to an actin binding site on MARCKS. (D) Protein kinase C phosphorylation of Ser29 inhibited the actin bundling activity of fascin. (E) Genetic screening in Drosophila identified two mutations that reduced (mutation of Gly) or eliminated (mutation of Ser) the actin bundling activity of fascin. Since Ser274 is on the other side on this particular view of the model, residues (Gln277-Asp280) nearby Ser274 are shown to indicate the location.

FIG. 13. Macroketone binding site overlaps with one of the actin binding site. (A) Residues His392 and His474 involved in macroketone binding were shown in blue. Other residues involved in actin binding were shown in orange (the N-terminal domain), in light blue (Ser39), or in red (Gly393). (B) Based on the cryo-EM model of fimbrin and actin filaments, a model of fascin and two actin filaments are proposed.

FIG. 14. Mutagenesis studies of residues involved in macroketone binding and in actin bundling. (A) Coomassie blue stain of purified fascin and its mutant

proteins. (B) Actin bundling assay for the wild-type fascin and its mutants. (C) Sensitivity to macroketone. Wild-type fascin, E391A and H474A mutants of fascin were assayed for their actin bundling activity in the absence or presence of macroketone.

FIG. 15 shows a diagram of a system used to carry out the instructions encoded by the storage medium of FIGs. 16 and 17.

FIG. 16 shows a cross section of a magnetic storage medium.

FIG. 17 shows a cross section of an optically-readable data storage medium.

Detailed Description of the Invention

The invention relates to compositions and methods for inhibiting fascin.

Definitions

An "effective amount" generally means an amount which provides the desired effect. For example, an effective dose is an amount sufficient to effect a beneficial or desired result. The dose could be administered in one or more administrations. The precise determination of what would be considered an effective dose may be based on factors individual to each subject, including size, age, injury (e.g., defect) or disease (e.g., defect) being treated and amount of time since the injury occurred or the disease began. One skilled in the art, particularly a physician, would be able to determine the effective dose. Doses can vary depending on the mode of administration, e.g., local or systemic; free or encapsulated. The effect can be inhibition of metastasis or other clinical endpoints, such as treatment, reduction or regression of metastatic cancer. Other effects can include reduction or inhibition of fascin mRNA expression and/or protein levels.

A "cell that expresses fascin" or a "cell expressing fascin" is any human or animal cell that expresses fascin. In some embodiments, the cell over-expresses fascin. Such a cell can, for example, be a cancer cell, a neuron, an immune cell, or an antigen presenting cell. The cancer cell can be any cancer or tumor cell associated with the cancers or tumors described herein. For example, the cancer cell can be a cancerous breast, ovarian, colon, pancreatic, esophageal, stomach, lung, bladder, carcinoma, lymphoma, sarcoma, melanoma, or astrocytoma cell.

The term "actin-binding site" as used herein means a fascin peptide or fascin peptidomimetic that includes one of two sites where actin is bound by fascin. One fascin actin-binding site includes fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250. The other fascin actin-binding site includes fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473.

The term "migrastatin analog binding site" as used herein means a fascin peptide or fascin peptidomimetic that includes the site where a migrstatin analog is bound by fascin. The mibrastatin binding site includes fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473. Actin can also bind to this site. While not wishing to be bound by any specific theory or mechanism, it is believed that migrastatin analogs inhibit the binding of actin to the migrastatin binding site.

The terms "small interfering RNA" or "siRNA" as used herein, refer to the mediators of RNAi, that is, RNA molecules capable of directing sequence-specific, post-transcriptional gene silencing of specific genes with which they share nucleotide sequence identity or similarity. In some organisms (e.g., *C. elegans*, *D. melanogaster* and various plants) these siRNAs can be created by the nucleolytic processing of longer dsRNAs. In mammalian cells they can also be produced from short (i.e., less than 30 base pairs) hairpin RNAs, or shRNAs.

The term "small hairpin siRNA," "short hairpin siRNA," or "shRNAs," as used herein, refers to small interfering RNAs (siRNAs) composed of a single strand of RNA that possesses regions of self-complementarity that cause the single strand to fold back upon itself and form a hairpin-like structure with an intramolecular duplexed region containing at least 19 base pairs. Because they are single-stranded, shRNAs can be readily expressed from single expression cassettes.

The term "fascin inhibitor" as used herein means a siRNA or an antisense RNA capable of hybridizing or binding to a fascin nucleic acid (e.g., a fascin mRNA with any of SEQ ID NO: 2, 4, 6 or 8), a small molecule (e.g., a migrastatin analog), an anti-fascin antibody that binds specifically to fascin (e.g., to a fascin

actin-binding site and/or to a fascin migrastatin binding site), a fascin peptide or fascin peptidomimetic that includes fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250, a fascin peptide or fascin peptidomimetic that includes fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473.

The phrase "inhibiting fascin expression or activity" as used herein means suppressing the fascin gene expression, interfering with translation of the fascin gene product, interfering with the fascin gene product function (e.g., by reversibly or irreversibly binding an inhibitor or by blocking or disrupting fascin interaction with cellular products such as actin), inactivating the fascin gene product (e.g., by reaction with an inactivating agent), or removing the fascin gene product (e.g., by fascin gene mutation or by tagging the fascin gene product for cellular destruction).

The term "knock down," as used herein, describes the condition where expression of a gene is reduced. For example, "knock down" can be created by mutation of a gene, deletion of a gene, or reduction in expression of a gene. One method for reducing expression of a gene involves RNAi, wherein the expression of a particular gene-product, or the cellular concentration of a particular RNA transcript, is reduced or eliminated by the sequence-specific, post-transcriptional gene silencing initiated by siRNAs that are homologous in sequence to the gene encoding said gene product. Hence, as used herein RNAi is a "knock down" agent.

A "subject" is a vertebrate, preferably a mammal, more preferably a human. Mammals include, but are not limited to, humans, farm animals, sport animals and pets. Included in the terms animals or pets are, but not limited to, dogs, cats, horses, rabbits, mice, rats, sheep, goats, cows and birds.

As used herein, "treat," "treating" or "treatment" includes treating, reversing, preventing, reducing, ameliorating, or inhibiting an injury or disease-related condition or a symptom of an injury or disease-related condition.

The terms "comprises", "comprising", and the like can have the meaning ascribed to them in U.S. Patent Law and can mean "includes", "including" and the

like. As used herein, "including" or "includes" or the like means including, without limitation.

Fascin

Fascin is an actin-bundling protein that has a major function in forming parallel actin bundles in cell protrusions such as lamellipodia, which are key specializations of the plasma membrane for cell migration (Adams 2004). Fascin mRNA is not usually expressed by normal epithelial cells, but its overexpression has been reported in many different types of carcinomas, including breast, ovary, colon, pancreas, esophagus, stomach, lung, and urinary bladder, as well as in other tumors, such as lymphomas, sarcomas, melanomas, and astrocytomas. The high expression of fascin mRNA is correlated with an aggressive clinical course and shorter survival. Fascin has been identified as the protein target of the migrastatin analogs described herein.

Fascin organizes actin into highly dynamic and architecturally diverse subcellular scaffolds. These scaffolds orchestrate a variety of mechanical processes, including filopodial protrusions in motile cells.

Sequences for fascin from a variety of sources are available. For example, publicly accessible databases of amino acid and nucleic acid sequences can be searched for fascin sequences. One example of a sequence for human fascin can be found in the database maintained by the National Center of Biotechnology Information at the www.ncbi.nlm.nih.gov website (accession number AAL01526, gi: 15625241), which is provided below as SEQ ID NO:1 for easy reference.

```
  1 MTANGTAEAV QIQFGLINCG NKYLTAEAFG FKVNASASSL
 41 KKKQIWTLEQ PPDEAGSAAV CLRSHLGRYL AADKDGNVTC
 81 EREVPGPDCR FLIVAHDDGR WSLQSEAHRR YFGGTEDRLS
121 CFAQTVSPAE KWSVHIAMHP QVNIYSVTRK RYAHLSARPA
161 DEIAVDRDVP WGVDSLITLA FQDQRYSVQT ADHRFLRHDG
201 RLVARPEPAT GYTLEFRSGK VAFRDCEGRY LAPSGPSGTL
241 KAGKATKVGK DELFALEQSC AQVVLQAANE RNVSTRQGMD
281 LSANQDEETD QETFQLEIDR DTKKCAFRTH TGKYWTLTAT
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321 GGVQSTASSK NASCYFDIEW RDRRITLRAS NGKFVTSKKN
361 GQLAASVETA GDSELFLMKL INRPIIVFRG EHGFIGCRKV
401 TGTLDANRSS YDVFQLEFND GAYNIKDSTG KYWTVGSDSA
441 VTSSGDTPVD FFFEFCDYNK VAIKVGGRYL KGDHAGVLKA
481 SAETVDPASL WEY
```

A genomic nucleotide sequence for the SEQ ID NO:1 fascin polypeptide is found, for example, at NCBI accession no. AY044229, gi: 15625240. A cDNA sequence for the SEQ ID NO:1 polypeptide can be found in the NCBI database as accession no. BC006304 (gi: 33873525). This nucleotide sequence is provided below for easy reference as SEQ ID NO:2.

```
   1 GCTGCGGAGG GTGCGTGCGG GCCGCGGCAG CCGAACAAAG
  41 GAGCAGGGGC GCCGCCGCAG GGACCCGCCA CCCACCTCCC
  81 GGGGCCGCGC AGCGGCCTCT CGTCTACTGC CACCATGACC
 121 GCCAACGGCA CAGCCGAGGC GGTGCAGATC CAGTTCGGCC
 161 TCATCAACTG CGGCAACAAG TACCTGACGG CCGAGGCGTT
 201 CGGGTTCAAG GTGAACGCGT CCGCCAGCAG CCTGAAGAAG
 241 AAGCAGATCT GGACGCTGGA GCAGCCCCCT GACGAGGCGG
 281 GCAGCGCGGC CGTGTGCCTG CGCAGCCACC TGGGCCGCTA
 321 CCTGGCGGCG GACAAGGACG GCAACGTGAC CTGCGAGCGC
 361 GAGGTGCCCG GTCCCGACTG CCGTTTCCTC ATCGTGGCGC
 401 ACGACGACGG TCGCTGGTCG CTGCAGTCCG AGGCGCACCG
 441 GCGCTACTTC GGCGGCACCG AGGACCGCCT GTCCTGCTTC
 481 GCGCAGACGG TGTCCCCCGC CGAGAAGTGG AGCGTGCACA
 521 TCGCCATGCA CCCTCAGGTC AACATCTACA GCGTCACCCG
 561 TAAGCGCTAC GCGCACCTGA GCGCGCGGCC GGCCGACGAG
 601 ATCGCCGTGG ACCGCGACGT GCCCTGGGGC GTCGACTCGC
 641 TCATCACCCT CGCCTTCCAG GACCAGCGCT ACAGCGTGCA
 681 GACCGCCGAC CACCGCTTCC TGCGCCACGA CGGGCGCCTG
 721 GTGGCGCGCC CCGAGCCGGC CACTGGCTAC ACGCTGGAGT
 761 TCCGCTCCGG CAAGGTGGCC TTCCGCGACT GCGAGGGCCG
 801 TTACCTGGCG CCGTCGGGGC CCAGCGGCAC GCTCAAGGCG
 841 GGCAAGGCCA CCAAGGTGGG CAAGGACGAG CTCTTTGCTC
 881 TGGAGCAGAG CTGCGCCCAG GTCGTGCTGC AGGCGGCCAA
 921 CGAGAGGAAC GTGTCCACGC GCCAGGGTAT GGACCTGTCT
 961 GCCAATCAGG ACGAGGAGAC CGACCAGGAG ACCTTCCAGC
1001 TGGAGATCGA CCGCGACACC AAAAAGTGTG CCTTCCGTAC
1041 CCACACGGGC AAGTACTGGA CGCTGACGGC CACCGGGGGC
1081 GTGCAGTCCA CCGCCTCCAG CAAGAATGCC AGCTGCTACT
1121 TTGACATCGA GTGGCGTGAC CGGCGCATCA CACTGAGGGC
1161 GTCCAATGGC AAGTTTGTGA CCTCCAAGAA GAATGGGCAG
1201 CTGGCCGCCT CGGTGGAGAC AGCAGGGGAC TCAGAGCTCT
1241 TCCTCATGAA GCTCATCAAC CGCCCCATCA TCGTGTTCCG
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1281 CGGGGAGCAT GGCTTCATCG GCTGCCGCAA GGTCACGGGC
1321 ACCCTGGACG CCAACCGCTC CAGCTATGAC GTCTTCCAGC
1361 TGGAGTTCAA CGATGGCGCC TACAACATCA AAGACTCCAC
1401 AGGCAAATAC TGGACGGTGG GCAGTGACTC CGTGGTCACC
1441 AGCAGCGGCG ACACTCCTGT GGACTTCTTC TTCGAGTTCT
1481 GCGACTATAA CAAGGTGGCC ATCAAGGTGG GCGGGCGCTA
1521 CCTGAAGGGC GACCACGCAG GCGTCCTGAA GGCCTCGGCG
1561 GAAACCGTGG ACCCCGCCTC GCTCTGGGAG TACTAGGGCC
1601 GGCCCGTCCT TCCCCGCCCC TGCCCACATG GCGGCTCCTG
1641 CCAACCCTCC CTGCTAACCC CTTCTCCGCC AGGTGGGCTC
1681 CAGGGCGGGA GGCAAGCCCC CTTGCCTTTC AAACTGGAAA
1721 CCCCAGAGAA AACGGTGCCC CCACCTGTCG CCCCTATGGA
1761 CTCCCCACTC TCCCCTCCGC CCGGGTTCCC TACTCCCCTC
1801 GGGTCAGCGG CTGCGGCCTG GCCCTGGGAG GGATTTCAGA
1841 TGCCCCTGCC CTCTTGTCTG CCACGGGGCG AGTCTGGCAC
1881 CTCTTTCTTC TGACCTCAGA CGGCTCTGAG CCTTATTTCT
1921 CTGGAAGCGG CTAAGGGACG GTTGGGGGCT GGGAGCCCTG
1961 GGCGTGTAGT GTAACTGGAA TCTTTTGCCT CTCCCAGCCA
2001 CCTCCTCCCA GCCCCCCAGG AGAGCTGGGC ACATGTCCCA
2041 AGCCTGTCAG TGGCCCTCCC TGGTGCACTG TCCCCGAAAC
2081 CCCTGCTTGG GAAGGGAAGC TGTCGGGTGG GCTAGGACTG
2121 ACCCTTGTGG TGTTTTTTTG GGTGGTGGCT GGAAACAGCC
2161 CCTCTCCCAC GTGGCAGAGG CTCAGCCTGG CTCCCTTCCC
2201 TGGAGCGGCA GGGCGTGACG GCCACAGGGT CTGCCCGCTG
2241 CACGTTCTGC CAAGGTGGTG GTGGCGGGCG GGTAGGGGTG
2281 TGGGGGCCGT CTTCCTCCTG TCTCTTTCCT TTCACCCTAG
2321 CCTGACTGGA AGCAGAAAAT GACCAAATCA GTATTTTTTT
2361 TAATGAAATA TTATTGCTGG AGGCGTCCCA GGCAAGCCTG
2401 GCTGTAGTAG CGAGTGATCT GGCGGGGGGC GTCTCAGCAC
2441 CCTCCCCAGG GGGTGCATCT CAGCCCCCTC TTTCCGTCCT
2481 TCCCGTCCAG CCCCAGCCCT GGGCCTGGGC TGCCGACACC
2521 TGGGCCAGAG CCCCTGCTGT GATTGGTGCT CCCTGGGCCT
2561 CCCGGGTGGA TGAAGCCAGG CGTCGCCCCC TCCGGGAGCC
2601 CTGGGGTGAG CCGCCGGGGC CCCCCCTGCT GCCAGCCTCC
2641 CCCGTCCCCA ACATGCATCT CACTCTGGGT GTCTTGGTCT
2681 TTTATTTTTT GTAAGTGTCA TTTGTATAAC TCTAAACGCC
2721 CATGATAGTA GCTTCAAACT GGAAATAGCG AAATAAAATA
2761 ACTCAGTCTG CAGCCCCAAA AAAAAAAAAA AAAAAAAAAA
```

One example of a sequence for human fascin 2 (accession no. NP_001070650, gi: 116295251) is provided below as SEQ ID NO:3:

```
 1 MPTNGLHQVL KIQFGLVNDT DRYLTAESFG FKVNASAPSL
41 KRKQTWVLEP DPGQGTAVLL RSSHLGRYLS AEEDGRVACE
81 AEQPGRDCRF LVLPQPDGRW VLRSEPHGRF FGGTEDQLSC
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 121 FATAVSPAEL WTVHLAIHPQ AHLLSVSRRR YVHLCPREDE
 161 MAADGDKPWG VDALLTLIFR SRRYCLKSCD SRYLRSDGRL
 201 VWEPEPRACY TLEFKAGKLA FKDCDGHYLA PVGPAGTLKA
 241 GRNTRPGKDE LFDLEESHPQ VVLVAANHRY VSVRQGVNVS
 281 ANQDDELDHE TFLMQIDQET KKCTFYSSTG GYWTLVTHGG
 321 IHATATQVSA NTMFEMEWRG RRVALKASNG RYVCMKKNGQ
 361 LAAISDFVGP PPRPAWTGKV AGGAAQQTLS PPGKDEEFTL
 401 KLINRPILVL RGLDGFVCHH RGSNQLDTNR SVYDVFHLSF
 441 SDGAYRIRGR DGGFWYTGSH GSVCSDGERA EDFVFEFRER
 481 GRLAIRARSG KYLRGGASGL LRADADAPAG TALWEY
```

A cDNA sequence for the SEQ ID NO:3 polypeptide can be found in the NCBI database as accession no. NM001077182 (gi: 116295250). This nucleotide sequence is provided below for easy reference as SEQ ID NO:4.

```
   1 GCAGGCAGGG GGTTCGTGAC GCCGGCTGGG TCTGGGGGCT
  41 GTGGGCCAGC CGAGCCGACC CGGGCTTCTG GGGGACCGCG
  81 GGGGCCGTGA GCACTCAGAG GGTGCATCCC AGGCCCCTCC
 121 GGGGACCCGG CCAGCCTGAA GATGCCGACG AACGGCCTGC
 161 ACCAGGTGCT GAAGATCCAG TTTGGCCTCG TCAACGACAC
 201 TGACCGCTAC CTGACAGCTG AGAGCTTCGG CTTCAAGGTC
 241 AATGCCTCGG CACCCAGCCT CAAGAGGAAG CAGACCTGGG
 281 TGCTGGAACC CGACCCAGGA CAAGGCACGG CTGTGCTGCT
 321 CCGCAGCAGC CACCTGGGCC GCTACCTGTC GGCAGAAGAG
 361 GACGGGCGCG TGGCCTGTGA GGCAGAGCAG CCGGGCCGTG
 401 ACTGCCGCTT CCTGGTCCTG CCGCAGCCAG ATGGGCGCTG
 441 GGTGCTGCGG TCCGAGCCGC ACGGCCGCTT CTTCGGAGGC
 481 ACCGAGGACC AGCTGTCCTG CTTCGCCACA GCCGTTTCCC
 521 CGGCCGAGCT GTGGACCGTG CACCTGGCCA TCCACCCGCA
 561 GGCCCACCTG CTGAGCGTGA GCCGGCGGCG CTACGTGCAC
 601 CTGTGCCCGC GGGAGGACGA GATGGCCGCA GACGGAGACA
 641 AGCCCTGGGG CGTGGACGCC CTCCTCACCC TCATCTTCCG
 681 GAGCCGACGG TACTGCCTCA AGTCCTGTGA CAGCCGCTAC
 721 CTGCGCAGCG ACGGCCGTCT GGTCTGGGAG CCTGAGCCCC
 761 GTGCCTGCTA CACGCTGGAG TTCAAGGCGG GCAAGCTGGC
 801 CTTCAAGGAC TGCGACGGCC ACTACCTGGC ACCCGTGGGG
 841 CCCGCAGGCA CCCTCAAGGC CGGCCGAAAC ACGCGACCTG
 881 GCAAGGATGA GCTCTTTGAT CTGGAGGAGA GTCACCCACA
 921 GGTGGTGCTG GTGGCTGCCA ACCACCGCTA CGTCTCTGTG
 961 CGGCAAGGGG TCAACGTCTC AGCCAATCAG GATGATGAAC
1001 TAGACCACGA GACCTTCCTG ATGCAAATTG ACCAGGAGAC
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1041 AAAGAAGTGC ACCTTCTATT CCAGCACTGG GGGCTACTGG
1081 ACCCTGGTCA CCCATGGGGG CATTCACGCC ACAGCCACAC
1121 AAGTTTCTGC CAACACCATG TTTGAGATGG AGTGGCGTGG
1161 CCGGCGGGTA GCACTCAAAG CCAGCAACGG GCGCTACGTG
1201 TGCATGAAGA AGAATGGGCA GCTGGCGGCT ATCAGCGATT
1241 TTGTCGGGCC CCCACCCCGC CCGGCCTGGA CAGGGAAGGT
1281 GGCGGGAGGG GCAGCGCAGC AGACGCTCTC CCCGCCAGGC
1321 AAGGACGAAG AGTTCACCCT CAAGCTCATC AACCGGCCCA
1361 TCCTGGTGCT GCGCGGCCTG GACGGCTTCG TCTGCCACCA
1401 CCGCGGCTCC AACCAGCTGG ACACCAACCG CTCCGTCTAC
1441 GACGTCTTCC ACCTGAGCTT CAGCGACGGC GCCTACCGGA
1481 TCCGAGGCCG CGACGGAGGG TTCTGGTACA CGGGCAGCCA
1521 CGGCAGCGTG TGCAGCGACG GCGAACGCGC CGAGGACTTC
1561 GTCTTCGAGT TCCGTGAGCG CGGCCGCCTG GCCATCCGCG
1601 CCCGGAGCGG CAAGTACCTG CGCGGCGGCG CCTCGGGCCT
1641 GCTGCGGGCC GATGCCGACG CCCCGGCCGG GACCGCGCTT
1681 TGGGAGTACT GAGGCCGCGC CCAGACCAGC CTGTCGCGCA
1721 TTAAAACCGT GTCTCTCCCG CAAAAAAAAA AAAAAAAAAA
1761 AA
```

One example of a sequence for human fascin 3 (accession no. NP_065102, gi: 9966791) is provided below as SEQ ID NO:5:

```
   1 MDETEWIHRH PKAEDLRVGL ISWAGTYLTF EACKNTVTAT
  41 AKSLGRRQTW EILVSNEHET QAVVRLKSVQ GLYLLCECDG
  81 TVCYGRPRTS HHGCFLLRFH RNSKWTLQCL ISGRYLESNG
 121 KDVFCTSHVL SAYHMWTPRP ALHVHVILYS PIHRCYARAD
 161 PTMGRIWVDA AVPCLEECGF LLHFRDGCYH LETSTHHFLS
 201 HVDRLFSQPS SQTAFHMQVR PGGLVALCDG EGGMLYPQGT
 241 HLLLGMGCNP MRGEEWFILQ HCPTWVSLRS KTGRFISVIY
 281 DGEVRAASER LNRMSLFQFE CDSESPTVQL RSANGYYLSQ
 321 RRHRAVMADG HPLESDTFFR MHWNCGRIIL QSCRGRFLGI
 361 APNSLLMANV ILPGPNEEFG ILFANRSFLV LRGRYGYVGS
 401 SSGHDLIQCN QDQPDRIHLL PCRPGIYHFQ AQGGSFWSIT
 441 SFGTFRPWGK FALNFCIELQ GSNLLTVLAP NGFYMRADQS
 481 GTLLADSEDI TRECIWEF
```

A cDNA sequence for the SEQ ID NO:5 fascin polypeptide can be found in the NCBI database as accession no. NM_020369 (gi: 9966790). This nucleotide sequence is provided below for easy reference as SEQ ID NO:6.

```
   1 CCCTTTCCCC ACTGTGGTGT GATAAGAGGC TGCCCTCACA
  41 GTCACAATGC TCCCGGGTCA CAGAGGTGCT GGGCCCCAGG
  81 CCAGCCTCTG CCTGGGAAGT TCTCTCTGGG AACATCTGGT
 121 GGGTACTACA GGCCCTATTC CAGGCCCTAT GGCCTGTGGA
 161 ACCTCACCAC GGGGGGGAGG GCTGGGCCAG ACGGAGACAT
 201 CACCTGTGGT GTCAGCCCCA TGGATGAGAC AGAGTGGATA
 241 CACAGACATC CCAAGGCTGA GGACCTAAGG GTTGGGCTCA
 281 TCAGCTGGGC AGGAACCTAC CTCACCTTTG AGGCATGCAA
 321 GAATACAGTC ACTGCAACTG CGAAGAGTTT GGGCAGGAGA
 361 CAGACCTGGG AGATCTTGGT GAGCAATGAG CATGAGACAC
 401 AGGCCGTGGT GCGACTAAAG AGCGTGCAGG GCCTCTACCT
 441 GCTGTGTGAG TGTGATGGCA CCGTGTGTTA TGGCCGCCCA
 481 AGGACCAGCC ACCATGGGTG CTTTCTACTG CGTTTCCACC
 521 GGAACAGCAA GTGGACCCTC CAGTGCCTAA TCTCTGGTCG
 561 TTATTTGGAG TCCAATGGCA AGGACGTGTT TTGCACTTCC
 601 CACGTCCTCT CAGCTTACCA CATGTGGACC CCCCGACCAG
 641 CCCTCCATGT CCACGTGATC CTCTACAGCC CCATCCACCG
 681 CTGCTATGCC CGGGCTGACC CCACTATGGG CCGCATCTGG
 721 GTGGACGCAG CAGTTCCCTG CCTGGAGGAG TGTGGCTTCC
 761 TGTTGCATTT CCGAGATGGA TGCTACCACC TGGAGACCTC
 801 TACACACCAC TTCTTGTCCC ATGTAGACCG GCTGTTCTCC
 841 CAACCCTCAT CACAGACAGC TTTTCACATG CAAGTGCGGC
 881 CTGGAGGGCT TGTGGCACTG TGTGATGGAG AAGGAGGCAT
 921 GTTATATCCA CAGGGCACGC ATCTGCTCTT GGGCATGGGC
 961 TGCAACCCCA TGAGGGGTGA GGAGTGGTTC ATCCTACAGC
1001 ACTGCCCAAC CTGGGTCAGC CTCAGGTCAA AGACTGGGCG
1041 GTTCATCTCA GTCATCTACG ATGGTGAGGT GCGTGCTGCT
1081 TCTGAGCGCT TAAACCGAAT GTCCTTGTTC CAGTTTGAAT
1121 GTGACAGTGA GAGCCCCACT GTGCAGCTTC GTTCAGCCAA
1161 TGGCTACTAC CTATCCCAGA GGCGCCACAG GGCAGTAATG
1201 GCTGATGGGC ACCCCCTGGA GTCTGACACG TTCTTCCGAA
1241 TGCACTGGAA CTGTGGCAGG ATCATCCTGC AGTCCTGCAG
1281 GGGGCGCTTC CTGGGCATTG CACCCAACAG CCTGCTGATG
1321 GCCAATGTCA TCCTTCCAGG CCCAAATGAG GAATTTGGGA
1361 TTTTATTTGC CAATCGCTCC TTCCTTGTAT TGCGAGGTCG
1401 TTATGGCTAT GTGGGCTCCT CATCGGGCCA TGACCTCATA
1441 CAGTGCAACC AGGATCAGCC CGACCGCATT CATCTACTAC
1481 CCTGCCGACC GGGTATCTAC CACTTCCAGG CACAGGGGGG
1521 ATCCTTCTGG TCAATAACAT CCTTTGGCAC CTTTCGCCCT
1561 TGGGGCAAGT TTGCCCTCAA CTTCTGTATC GAGCTTCAGG
1601 GGAGCAACTT ACTCACTGTA CTGGCCCCCA ATGGCTTCTA
1641 CATGCGAGCC GACCAAAGTG GCACCCTGTT GGCAGACAGT
1681 GAAGACATTA CCAGAGAGTG TATCTGGGAA TTTTAGGTCA
1721 ATGGGATGTC ACCTACCAAA ATCCAAATCC TCCAGGAAAA
1761 ACTACTACAC TAAATGGACC AGGAACCTCA GAGTCAAGAT
1801 CCAAGAGAAG AACATCTGTT ACAACTTTTC CTACCCAGTT
1841 TAGCAAAACA CCTGTTTTAT GCAACAATAC ATCACAACAG
```

1881 GCC

One example of a sequence for mouse fascin homolog 1 (accession number NP 032010, gi: 113680348) is provided below as SEQ ID NO:7:

```
   1 MTANGTAEAV QIQFGLISCG NKYLTAEAFG FKVNASASSL
  41 KKKQIWTLEQ PPDEAGSAAV CLRSHLGRYL AADKDGNVTC
  81 EREVPDGDCR FLVVAHDDGR WSLQSEAHRR YFGGTEDRLS
 121 CFAQSVSPAE KWSVHIAMHP QVNIYSVTRK RYAHLSARPA
 161 DEIAVDRDVP WGVDSLITLA FQDQRYSVQT SDHRFLRHDG
 201 RLVARPEPAT GFTLEFRSGK VAFRDCEGRY LAPSGPSGTL
 241 KAGKATKVGK DELFALEQSC AQVVLQAANE RNVSTRQGMD
 281 LSANQDEETD QETFQLEIDR DTRKCAFRTH TGKYWTLTAT
 321 GGVQSTASTK NASCYFDIEW CDRRITLRAS NGKFVTAKKN
 361 GQLAASVETA GDSELFLMKL INRPIIVFRG EHGFIGCRKV
 401 TGTLDANRSS YDVFQLEFND GAYNIKDSTG KYWTVGSDSS
 441 VTSSSDTPVD FFLEFCDYNK VALKVGGRYL KGDHAGVLKA
 481 CAETIDPASL WEY
```

A cDNA sequence for the SEQ ID NO:7 fascin polypeptide can be found in the NCBI database as accession no. NM_007984 (gi: 113680347). This nucleotide sequence is provided below for easy reference as SEQ ID NO:8.

```
   1 TGTGGAGAAC TGCAGCGGGC TAAGCCGTGT TGAACAAAGG
  41 AGGTCGGGCA CAGCTATCCA AGCTCCCGGG GCCACCGGGC
  81 CGCCCTCCGC CACCATGACC GCCAACGGCA CGGCAGAGGC
 121 TGTGCAGATT CAGTTCGGGC TCATCAGCTG CGGCAACAAG
 161 TACCTGACAG CCGAGGCGTT CGGGTTCAAG GTGAACGCAT
 201 CCGCTAGTAG CTTGAAAAAG AAGCAGATCT GGACGCTGGA
 241 GCAACCTCCC GATGAGGCGG GCAGCGCGGC CGTGTGTCTG
 281 CGCAGCCACC TGGGTCGCTA CCTGGCCGCC GACAAGGACG
 321 GCAACGTGAC CTGCGAGCGC GAGGTGCCCG ACGGCGACTG
 361 CCGCTTTCTC GTCGTGGCGC ACGACGACGG CCGCTGGTCG
 401 CTGCAGTCCG AGGCTCACCG GCGCTACTTT GGCGGCACCG
 441 AGGACCGCCT GTCCTGCTTC GCGCAGAGCG TGTCGCCGGC
 481 CGAGAAGTGG AGCGTGCACA TCGCCATGCA CCCGCAGGTT
 521 AACATCTACA GCGTTACCCG CAAGCGCTAC GCGCATCTGA
 561 GCGCGCGGCC GGCCGACGAG ATCGCGGTAG ACCGCGACGT
 601 GCCTTGGGGC GTCGACTCGC TCATCACCTT GGCCTTCCAG
 641 GACCAACGCT ACAGTGTGCA GACGTCCGAC CACCGCTTCC
 681 TGCGCCACGA CGGGCGCCTT GTGGCACGGC CGGAGCCCGC
 721 CACGGGCTTC ACGCTGGAGT TCCGCTCCGG CAAGGTGGCC
 761 TTTCGCGACT GCGAAGGTCG CTACCTGGCT CCGTCCGGGC
 801 CCAGCGGCAC CCTCAAGGCT GGCAAGGCCA CCAAGGTGGG
 841 CAAAGATGAG CTCTTCGCCC TGGAACAGAG CTGCGCTCAG
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 881 GTGGTGCTGC AGGCGGCCAA CGAGAGGAAC GTGTCCACGC
 921 GCCAGGGAAT GGACCTGTCA GCCAATCAGG ATGAAGAGAC
 961 CGATCAGGAG ACCTTCCAGC TGGAGATCGA CCGCGACACA
1001 AGAAAGTGTG CCTTTCGCAC CCACACGGGC AAGTACTGGA
1041 CACTGACGGC GACCGGAGGT GTGCAATCCA CTGCGTCCAC
1081 CAAGAACGCC AGCTGCTACT TTGACATCGA GTGGTGTGAC
1121 CGCCGGATCA CTCTGAGAGC CTCCAACGGC AAGTTTGTGA
1161 CCGCCAAGAA AAATGGCCAG CTGGCCGCCT CGGTGGAGAC
1201 AGCAGGGGAC TCGGAACTCT TCCTCATGAA GCTGATTAAC
1241 CGCCCCATCA TCGTGTTCCG GGGGGAACAC GGGTTCATTG
1281 GCTGCCGCAA GGTCACGGGC ACTCTGGATG CCAACCGTTC
1321 CAGTTACGAT GTCTTCCAGT TGGAATTCAA TGACGGCGCC
1361 TACAACATCA AAGACTCCAC GGGCAAGTAC TGGACGGTGG
1401 GTAGTGATTC CTCGGTCACC AGCAGCAGCG ACACCCCTGT
1441 GGATTTCTTC CTTGAGTTCT GTGACTACAA TAAGGTGGCT
1481 CTCAAGGTGG GCGGCCGCTA CCTGAAGGGG GACCACGCTG
1521 GGGTCCTGAA GGCCTGCGCG GAGACTATCG ACCCCGCCTC
1561 ACTCTGGGAG TACTAGGGCC ACCTGCCCTC TGCAGGCCGC
1601 TCTCGTCAGT CCCTCCTGTT ATCCTTACTC ATCGGGTGGC
1641 CCTGCAGCAG GTGGCAAACC CCTTGCCTTT CAAACTGGAA
1681 ACCCAAGAGA AAACGGTGCC CTTGCTGTCA CCCTCTGTGG
1721 ACCCCTTTTC CCTAACTCAC TGCTCCCCAT GGGTCGGTGG
1761 CTGCAGACTG TCCCCAGGAG GGACTCTGGT TCCCTCTGTC
1801 CCCTTCTTTC CATGGGGAAC TCTGGCACCT TTCTTCTGAC
1841 CTCAGTCAAC TCTGAGCCTT ATTTCCCCCC AGGAAGTGGC
1881 CTAGGAGAAG CTACAGGGCC TAGGGACTTA CCCTGAGCTT
1921 GTAACTGGAA GACCCCGTCC CTATCCCCGC TCCCGCCCCC
1961 ACCCCACCCC ACCCCTGCTC TGGCCCCAGC CTCTGGAGGC
2001 CAGCCTTTTG GCGGGACTGA AGCCGGGCAT GGCCAACCTT
2041 GCCCACAAGT GTTTTTCTGG ATCTTGGCTG GAAGGCAGTC
2081 TGTCCCATCC TGCAGTGTTT GGGCCTGGCT CTTTGACTCA
2121 AAGCTAGCTA GGTGGCACTC CGTGTCGCTC CTGCACATTC
2161 TGGAAGGGGC GGGCCTCTCA CCCACCTCAT TCCTTTTCCC
2201 CCTGGCCTGA CTGGAAGCAG AAAAATGACC AAATCAGTAT
2241 TTTTTTTTTT TTCTTTAAGG AAATGTTACT GTTGAAAGGC
2281 CCTAGGCAAG CCTGCCCTGT TGGTTGTAGT CGTGAGTGGT
2321 CTTGGGGGGA GATGCTTGGC TCCTGTCCCT GCCTCCCCAG
2361 CGGGTTCCCT CCCTCCCTCC TGCCTGACCA CCCCAGCTCT
2401 GGCTCTGTGA TTGGTGCTCC ACGTCTTCCC AGACACCTCG
2441 GGGCTCCTGG GCGGGAGAAA GCCGGATGTG CCCCTCCCTG
2481 GGAGCCCTGG AGTAAACCTC AGGGGGCCCT TTCCCAATCA
2521 CCCCCTTCCA CCGACCCCTC AACACCATGC ATCTCACTCT
2561 GGGTGTCTCG CTCCTTTATT TTTTTGTAAC TGTCATTTCT
2601 ATAACTCTGA AGACCCATGA TAGTAAGCTT TGAACTGGAA
2641 AATAAAGTAA AATCAAGTCT GCGGCCC
```

In some embodiments, the fascin polypeptide is a truncated polypeptide that includes the actin binding site and/or the binding site for migrastatin analogs. As illustrated in more detail below, fascin binds migrastatin analogs and the fascin binding site for such migrastatin analogs includes fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473. Moreover, fascin also has two actin binding sites. One of these two sites is located in the same cleft as the binding site for migrastatin analogs. The second actin binding includes amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250.

One example of a truncated fascin polypeptide that can be used in the invention is any fascin peptide having fascin amino acids 259 through 493, which can fold properly to generate the actin and/or migrastatin binding sites. Thus, for example, a fascin peptide having amino acids 259 through 493 of SEQ ID NO:1 has the following sequence (SEQ ID NO:9).

```
259                       SC AQVVLQAANE RNVSTRQGMD
281 LSANQDEETD QETFQLEIDR DTKKCAFRTH TGKYWTLTAT
321 GGVQSTASSK NASCYFDIEW RDRRITLRAS NGKFVTSKKN
361 GQLAASVETA GDSELFLMKL INRPIIVFRG EHGFIGCRKV
401 TGTLDANRSS YDVFQLEFND GAYNIKDSTG KYWTVGSDSA
441 VTSSGDTPVD FFFEFCDYNK VAIKVGGRYL KGDHAGVLKA
481 SAETVDPASL WEY
```

Another example, of a fascin peptide having amino acids 259 through 493 of SEQ ID NO:3 has the following sequence (SEQ ID NO:10).

```
259                       PQ VVLVAANHRY VSVRQGVNVS
281 ANQDDELDHE TFLMQIDQET KKCTFYSSTG GYWTLVTHGG
321 IHATATQVSA NTMFEMEWRG RRVALKASNG RYVCMKKNGQ
361 LAAISDFVGP PPRPAWTGKV AGGAAQQTLS PPGKDEEFTL
401 KLINRPILVL RGLDGFVCHH RGSNQLDTNR SVYDVFHLSF
441 SDGAYRIRGR DGGFWYTGSH GSVCSDGERA EDFVFEFRER
```

481 GRLAIRARSG KYLRGGASGL LRADADAPAG TALWEY

Another example, of a fascin peptide having amino acids 259 through 493 of SEQ ID NO:5 has the following sequence (SEQ ID NO:11).

259 LQ HCPTWVSLRS KTGRFISVIY
281 DGEVRAASER LNRMSLFQFE CDSESPTVQL RSANGYYLSQ
321 RRHRAVMADG HPLESDTFFR MHWNCGRIIL QSCRGRFLGI
361 APNSLLMANV ILPGPNEEFG ILFANRSFLV LRGRYGYVGS
401 SSGHDLIQCN QDQPDRIHLL PCRPGIYHFQ AQGGSFWSIT
441 SFGTFRPWGK FALNFCIELQ GSNLLTVLAP NGFYMRADQS
481 GTLLADSEDI TRECIWEF

Another example, of a fascin peptide having amino acids 259 through 493 of SEQ ID NO:7 has the following sequence (SEQ ID NO:12).

259 SC AQVVLQAANE RNVSTRQGMD
281 LSANQDEETD QETFQLEIDR DTRKCAFRTH TGKYWTLTAT
321 GGVQSTASTK NASCYFDIEW CDRRITLRAS NGKFVTAKKN
361 GQLAASVETA GDSELFLMKL INRPIIVFRG EHGFIGCRKV
401 TGTLDANRSS YDVFQLEFND GAYNIKDSTG KYWTVGSDSS
441 VTSSSDTPVD FFLEFCDYNK VALKVGGRYL KGDHAGVLKA
481 CAETIDPASL WEY

Such fascin peptides are useful as therapeutic agents and as antigens for generating anti-fascin antibodies. As illustrated and described herein, metastatic cancer is associated with increased expression and/or activity of fascin. Thus, agents that compete with or inhibit fascin expression and fascin activity are useful therapeutic agents for treating cancer, particularly metastatic cancer. For example, peptides having fascin amino acids 259 through 493 can compete with fascin in vivo and can inhibit endogenous fascin performing its usual role in promoting cancer metastasis. Moreover, administration of peptides having fascin amino acids 259 through 493 can immunize the mammal against endogenously produced fascin, particularly against the actin and/or migrastatin binding sites of fascin. Antibodies generated in the immunized animals serve to prevent fascin from binding to actin.

Alternatively, such antibodies can mimic the inhibitory effects of migrastatin analogs by binding to the migrastatin binding site of fascin.

Inhibitory Nucleic Acids

Nucleic acids that can inhibit the expression and/or translation of fascin can be employed in the methods of the invention described herein. Such an inhibitory nucleic acid can bind to a fascin nucleic acid, for example, a fascin RNA with a sequence corresponding to any of SEQ ID NOs: 2, 4, 6, or 8. An inhibitory nucleic acid is a polymer of ribose nucleotides or deoxyribose nucleotides having more than three nucleotides in length. An inhibitory nucleic acid may include naturally-occurring nucleotides; synthetic, modified, or pseudo-nucleotides such as phosphorothiolates; as well as nucleotides having a detectable label such as ^{32}P, biotin, fluorescent dye or digoxigenin. An inhibitory nucleic acid that can reduce the expression and/or activity of a fascin nucleic acid may be completely complementary to the fascin nucleic acid. Alternatively, some variability between the sequences may be permitted.

An inhibitory nucleic acid of the invention can hybridize to a fascin nucleic acid (e.g., any of SEQ ID NOs: 2, 4, 6, or 8) under intracellular conditions or under stringent hybridization conditions. The inhibitory nucleic acids of the invention are sufficiently complementary to endogenous fascin nucleic acids to inhibit expression of a fascin nucleic acid under either or both conditions. Intracellular conditions refer to conditions such as temperature, pH and salt concentrations typically found inside a cell, e.g. a mammalian cell. One example of such a mammalian cell is a cancer cell (e.g., a metastatic cell), or any cell where fascin is or may be expressed.

Generally, stringent hybridization conditions are selected to be about 5°C lower than the thermal melting point (T_m) for the specific sequence at a defined ionic strength and pH. However, stringent conditions encompass temperatures in the range of about 1°C to about 20°C lower than the thermal melting point of the selected sequence, depending upon the desired degree of stringency as otherwise qualified herein. Inhibitory nucleic acids that comprise, for example, 2, 3, 4, or 5 or more stretches of contiguous nucleotides that are precisely complementary to a

fascin coding sequence, each separated by a stretch of contiguous nucleotides that are not complementary to adjacent coding sequences, may inhibit the function of a fascin nucleic acid. In general, each stretch of contiguous nucleotides is at least 4, 5, 6, 7, or 8 or more nucleotides in length. Non-complementary intervening sequences may be 1, 2, 3, or 4 nucleotides in length. One skilled in the art can easily use the calculated melting point of an inhibitory nucleic acid hybridized to a sense nucleic acid to estimate the degree of mismatching that will be tolerated for inhibiting expression of a particular target nucleic acid. Inhibitory nucleic acids of the invention include, for example, a ribozyme or an antisense nucleic acid molecule.

An antisense nucleic acid molecule may be single or double stranded (e.g. a small interfering RNA (siRNA)), and may function in an enzyme-dependent manner or by steric blocking. Antisense molecules that function in an enzyme-dependent manner include forms dependent on RNase H activity to degrade target mRNA. These include single-stranded DNA, RNA and phosphorothioate molecules, as well as the double-stranded RNAi/siRNA system that involves target mRNA recognition through sense-antisense strand pairing followed by degradation of the target mRNA or by the RNA-induced silencing complex. Steric blocking antisense, which are RNase-H independent, interferes with gene expression or other mRNA-dependent cellular processes by binding to a target mRNA and getting in the way of other processes. Steric blocking antisense includes 2'-O alkyl (usually in chimeras with RNase-H dependent antisense), peptide nucleic acid (PNA), locked nucleic acid (LNA) and morpholino antisense.

Small interfering RNAs, for example, may be used to specifically reduce fascin translation such that the level of fascin polypeptide is reduced. siRNAs mediate post-transcriptional gene silencing in a sequence-specific manner. See, for example, http://www.ambion.com/techlib/hottopics/rnai/rnai _may2002_print.html (last retrieved May 10, 2006). Once incorporated into an RNA-induced silencing complex, siRNAs mediate cleavage of the homologous endogenous mRNA transcript by guiding the complex to the homologous mRNA transcript, which is then cleaved by the complex. The siRNA may be homologous to any region of the

fascin transcript. The region of homology may be 30 nucleotides or less in length, preferably less than 25 nucleotides, more preferably about 21 to 23 nucleotides, most preferably about 19 nucleotides in length. SiRNA is typically double stranded and may have two-nucleotide 3' overhangs, for example, 3' overhanging UU dinucleotides. Methods for designing siRNAs are known to those skilled in the art. See, for example, Elbashir *et al. Nature* 411: 494-498 (2001); Harborth *et al. Antisense Nucleic Acid Drug Dev.* 13: 83-106 (2003). Typically, a target site that begins with AA, has 3' UU overhangs for both the sense and antisense siRNA strands, and has an approximate 50 % G/C content. siRNAs may be chemically synthesized, created by *in vitro* transcription, or expressed from an siRNA expression vector or a PCR expression cassette. See, e.g., http://www.ambion.com/techlib/tb/tb_506html (last retrieved May 10, 2006). Chemically synthesized siRNA relies on the same solid-phase support chemistry used to generate DNA primers for PCR. Expression or viral vectors and their RNA polymerase III (Pol III) promoters drive the expression of either siRNA transcripts, as separate sense and antisense strands that anneal in the cell, or a single short hairpin RNA transcript (Paddison,P.J. et al.(2002) Genes Dev.16,948-958; Sui, G. et al.(2002) Proc. Natl. Acad. Sci. U.S.A. 99, 6047-6052; Paul,C.P. et al. (2002) Nat. Biotechnol.20,505-508; Miyagishi M, et al. (2002) Nat. Biotechnol.20, 497-500). Human and mouse U6 and the human H1 are the most commonly used RNA polymerase III promoters. The polymerase III enzyme initiates and terminates RNA transcripts at well-defined positions (Goomer RS, et al. (1992) Nucleic Acids Res. Sep 25;20(18):4903-12) making its promoters well suited for the synthesis of siRNA or shRNA.

The short length of these Pol III promoters (less than 300 bp) facilitates the generation of expression cassettes using PCR methods to amplify a linear fragment of double-stranded DNA containing the necessary promoters and the siRNA or shRNA sequence (Catanotto, D. et al.(2002) RNA 8, 1454-1460). Either the cassette itself or the purified in vitro transcript of the cassette serves as the source of nucleic acid for RNAi.

Finally, treatment of dsRNA in vitro with purified mammalian Dicer or the E. coli enzyme RNase III digests the nucleic acid into a population of siRNA duplexes. Generation of the dsRNA involves the in vitro transcription of both strands of either a gene-specific fragment or a full-length cDNA of the gene of interest cloned into an appropriate vector.

When an siRNA is expressed from an expression vector or a PCR expression cassette, the insert encoding the siRNA may be expressed as an RNA transcript that folds into an siRNA hairpin. Thus, the RNA transcript may include a sense siRNA sequence that is linked to its reverse complementary antisense siRNA sequence by a spacer sequence that forms the loop of the hairpin as well as a string of U's at the 3' end. The loop of the hairpin may be of any appropriate lengths, for example, 3 to 30 nucleotides in length, preferably, 3 to 23 nucleotides in length, and may be of various nucleotide sequences including, AUG, CCC, UUCG, CCACC, CTCGAG, AAGCUU, CCACACC and UUCAAGAGA. SiRNAs also may be produced *in vivo* by cleavage of double-stranded RNA introduced directly or via a transgene or virus. Amplification by an RNA-dependent RNA polymerase may occur in some organisms.

Table 1 illustrates siRNA target sequences of human fascin useful in the invention described herein.

Table 1

siRNA Target Sequence	SEQ ID NO:
CCAGCAGCCTGAAGAAGAA	13
GGCAAGTACTGGACGCTGA	14
CAAAGACTCCACAGGCAAA	15
ATAACAAGGTGGCCATCAA	16
CTGAAGGCCTCGGCGGAAA	17
TCAAAGACTCCACAGGCAA	18
AGACCGACCAGGAGACCTT	19
CTGAAGAAGAAGCAGATCT	20
CCTTCCAGGACCAGCGCTA	21
CCAAGGTGGGCAAGGACGA	22
ACTATAACAAGGTGGCCAT	23
GCGTTCGGGTTCAAGGTGA	24
GCCAGCAGCCTGAAGAAGA	25
AAGAAGAAGCAGATCTGGA	26

siRNA Target Sequence	SEQ ID NO:
GTCAACATCTACAGCGTCA	27
GTATGGACCTGTCTGCCAA	28
GCGCCTACAACATCAAAGA	29
GCGACACTCCTGTGGACTT	30
CCGCCAGCAGCCTGAAGAA	31
AGAAGTGGAGCGTGCACAT	32
TGGGCAAGGACGAGCTCTT	33
GCCTGAAGAAGAAGCAGAT	34
CCAATCAGGACGAGGAGAC	35
GAGGAGACCGACCAGGAGA	36
AGATCGACCGCGACACCAA	37
GAGCATGGCTTCATCGGCT	38
TGTCCACGCGCCAGGGTAT	39
GCTGCTACTTTGACATCGA	40
GGCAAATACTGGACGGTGG	41
AGCCTGAAGAAGAAGCAGA	42
GGTATGGACCTGTCTGCCA	43
CTGCCAATCAGGACGAGGA	44
TTTGTGACCTCCAAGAAGA	45
ACGCCAACCGCTCCAGCTA	46
CCTACAACATCAAAGACTC	47
ATCAAAGACTCCACAGGCA	48
AGTTCTGCGACTATAACAA	49
GACAAGGACGGCAACGTGA	50
AGGTCAACATCTACAGCGT	51
ACGAGGAGACCGACCAGGA	52
GCAAGTTTGTGACCTCCAA	53
TGAAGAAGAAGCAGATCTG	54
TCGAGTTCTGCGACTATAA	55
AGATCTGGACGCTGGAGCA	56
GCCTACAACATCAAAGACT	57
CTTCGAGTTCTGCGACTAT	58
ACCCTCAGGTCAACATCTA	59
TCAACTGCGGCAACAAGTA	60
CTGGAGATCGACCGCGACA	61
CCTCCAAGAAGAATGGGCA	62

An antisense inhibitory nucleic acid may also be used to specifically reduce fascin expression, for example, by inhibiting transcription and/or translation. An antisense inhibitory nucleic acid is complementary to a sense nucleic acid encoding fascin. For example, it may be complementary to the coding strand of a double-

stranded cDNA molecule or complementary to an mRNA sequence. It may be complementary to an entire coding strand or to only a portion thereof. It may also be complementary to all or part of the noncoding region of a nucleic acid encoding fascin. The non-coding region includes the 5' and 3' regions that flank the coding region, for example, the 5' and 3' untranslated sequences. An antisense inhibitory nucleic acid is generally at least six nucleotides in length, but may be about 8, 12, 15, 20, 25, 30, 35, 40, 45, or 50 nucleotides long. Longer inhibitory nucleic acids may also be used.

An antisense inhibitory nucleic acid may be prepared using methods known in the art, for example, by expression from an expression vector encoding the antisense inhibitory nucleic acid or from an expression cassette. Alternatively, it may be prepared by chemical synthesis using naturally-occurring nucleotides, modified nucleotides or any combinations thereof. In some embodiments, the inhibitory nucleic acids are made from modified nucleotides or non-phosphodiester bonds, for example, that are designed to increase biological stability of the inhibitory nucleic acid or to increase intracellular stability of the duplex formed between the antisense inhibitory nucleic acid and the sense nucleic acid.

Naturally-occurring nucleotides include the ribose or deoxyribose nucleotides adenosine, guanine, cytosine, thymine and uracil.

Examples of modified nucleotides include 5-fluorouracil, 5-bromouracil, 5-chlorouracil, 5-iodouracil, hypoxanthine, xanthine, 4-acetylcytosine, 5-(carboxyhydroxylmethyl) uracil, 5-carboxymethylaminomethyl-2-thiouridine, 5-carboxymethylaminomethyluracil, dihydrouracil, beta-D-galactosylqueosine, inosine, N6-isopentenyladenine, 1-methylguanine, 1-methylinosine, 2,2-dimethylguanine, 2-methyladenine, 2-methylguanine, 3-methylcytosine, 5-methylcytosine, N6-adenine, 7-methylguanine, 5-methylaminomethyluracil, 5-methoxyaminomethyl-2-thiouracil, beta-D-mannosylqueosine, 5'-methoxycarboxymethyluracil, 5-methoxyuracil, 2-methythio-N6-isopentenyladeninje, uracil-5oxyacetic acid, butoxosine, pseudouracil, queosine, 2-thiocytosine, 5-methyl-2-thiouracil, 2-thiouracil, 4-thiouracil, 5-methyluracil, uracil-

5-oxacetic acid methylester, uracil-5-oxacetic acid, 5-methyl-2-thiouracil, 3-(3-amino-3-N-2-carboxypropyl) uracil, (acp3)w, and 2,6-diaminopurine.

An inhibitor of the invention can also be a small hairpin RNA or short hairpin RNA (shRNA) is a sequence of RNA that makes a tight hairpin turn that can be used to silence gene expression via RNA interference. The shRNA hairpin structure is cleaved by the cellular machinery into an siRNA, which is then binds to and cleaves the target mRNA. shRNA can be introduced into cells via a vector encoding the shRNA, where the shRNA coding region is operably linked to a promoter. The selected promoter permits expression of the shRNA. For example, the promoter can be a U6 promoter, which is useful for continuous expression of the shRNA. The vector can, for example, be passed on to daughter cells, allowing the gene silencing to be inherited. *See,* McIntyre G, Fanning G, *Design and cloning strategies for constructing shRNA expression vectors*, BMC BIOTECHNOL. 6:1 (2006); Paddison et al., *Short hairpin RNAs (shRNAs) induce sequence-specific silencing in mammalian cells*, GENES DEV. 16 (8): 948–58 (2002).

An inhibitor of the invention may also be a ribozyme. A ribozyme is an RNA molecule with catalytic activity and is capable of cleaving a single-stranded nucleic acid such as an mRNA that has a homologous region. *See*, for example, Cech, Science 236: 1532-1539 (1987); Cech, Ann. Rev. Biochem. 59:543-568 (1990); Cech, Curr. Opin. Struct. Biol. 2: 605-609 (1992); Couture and Stinchcomb, Trends Genet. 12: 510-515 (1996). A ribozyme may be used to catalytically cleave a fascin mRNA transcript and thereby inhibit translation of the mRNA. See, for example, Haseloff *et al.*, U.S. Pat. No. 5,641,673.

Methods of designing and constructing a ribozyme that can cleave an RNA molecule in trans in a highly sequence specific manner have been developed and described in the art. See, for example, Haseloff *et al.*, Nature 334:585-591 (1988). A ribozyme may be targeted to a specific RNA by engineering a discrete "hybridization" region into the ribozyme. The hybridization region contains a sequence complementary to the target RNA that enables the ribozyme to specifically hybridize with the target. See, for example, Gerlach *et al.*, EP 321,201. The target sequence may be a segment of about 5, 6, 7, 8, 9, 10, 12, 15, 20, or 50

contiguous nucleotides selected from a specific nucleotide sequence. Longer complementary sequences may be used to increase the affinity of the hybridization sequence for the target.

The hybridizing and cleavage regions of the ribozyme can be integrally related; thus, upon hybridizing to the target RNA through the complementary regions, the catalytic region of the ribozyme can cleave the target. Thus, an existing ribozyme may be modified to target a fascin nucleic acid of the invention by modifying the hybridization region of the ribozyme to include a sequence that is complementary to the target fascin nucleic acid. Alternatively, an mRNA encoding a fascin may be used to select a catalytic RNA having a specific ribonuclease activity from a pool of RNA molecules. See, for example, Bartel & Szostak, Science 261:1411-1418 (1993).

Thus, inhibitory nucleic acids of the invention may include modified nucleotides, as well as natural nucleotides such as combinations of ribose and deoxyribose nucleotides, and an antisense inhibitory nucleic acid of the invention may be of any length discussed above and that is complementary to fascin.

In some embodiments, expression cassettes are employed in the various embodiments described herein. Expression cassettes can be of any suitable construction, and can be included in any appropriate delivery vector. Such delivery vectors include plasmid DNA, viral DNA, and the like. The means by which the expression cassette in its delivery or expression vector is introduced into target cells or target organism can be transfection, reverse transfection, virus induced transfection, electroporation, direct introduction by biolystics (e.g., using a "gene gun;" BioRad, Inc., Emeryville, Calif.), and the like. Other methods that can be employed include methods widely known in the art as the methods of gene therapy. Once delivered into a target cell, or target organism the expression cassette may be maintained on an autonomously replicating piece of DNA (e.g., an expression vector), or may be integrated into the genome of the target cell or target organism.

Typically, to assemble the expression cassettes and vectors of the present invention a nucleic acid, preferably a DNA, encoding an siRNA is incorporated into a unique restriction endonuclease cleavage site, or a multiple cloning site, within a

pre-existing "empty" expression cassette to form a complete recombinant expression cassette that is capable of directing the production of the siRNA transcripts of the present invention. Frequently such complete recombinant expression cassettes reside within, or inserted into, expression vectors designed for the expression of such siRNA transcripts. Methods for the construction of an expression vector for purposes of this invention should be apparent to skilled artisans apprised of the present invention. (See generally, Current Protocols in Molecular Biology, Vol. 2, Ed. Ausubel, et al., Greene Publish. Assoc. & Wiley Interscience, Ch. 13, 1988; Glover, DNA Cloning, Vol. II, IRL Press, Wash., D.C., Ch. 3, 1986; Bitter, et al., in Methods in Enzymology 153:516-544 (1987); The Molecular Biology of the Yeast Saccharomyces, Eds. Strathern et al., Cold Spring Harbor Press, Vols. I and II, 1982; and Sambrook et al., Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Press, 1989.)

Generally, the expression cassettes inserted or assembled within the expression vectors have a promoter operably linked to a DNA encoding the siRNA that is to be employed. The promoter can be a native promoter, i.e., a promoter that is responsible for the expression of that particular gene product in cells, or it can be any other suitable promoter. Alternatively, the expression cassette can be a chimera, i.e., having a heterologous promoter that is not the native promoter responsible for the expression of the siRNA. Such heterologous promoters can even be from a different species than the target cell or organism.

The expression vector may further include an origin of DNA replication for the replication of the vectors in target cells. Preferably, the expression vectors also include a replication origin for the amplification of the vectors in, e.g., E. coli, and selection marker(s) for selecting and maintaining only those target cells harboring the expression vectors. Additionally, in some embodiments the expression vectors also contain inducible or derepressible promoters, which function to control the transcription of the siRNA transcript from the DNA that encodes it. Other regulatory sequences such as transcriptional enhancer sequences and translation regulation sequences (e.g., Shine-Dalgarno sequence) can also be operably included in the expression vectors. Transcription termination sequences, and polyadenylation

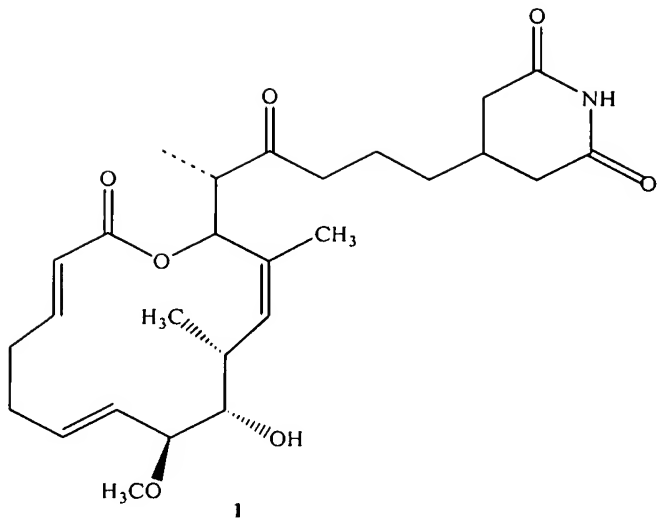
signal sequences, such as those from bovine growth hormone, SV40, lacZ and AcMNPV polyhedral protein genes, may also be present.

The expression vectors of the present invention can be introduced into the target cells by any techniques known in the art, e.g., by direct DNA transformation, microinjection, electroporation, viral infection, lipofection, biolystics, and the like. The expression of the siRNA can be transient or stable, inducible or derepressible. The expression vectors can be maintained in target cells in an extrachromosomal state, i.e., as self-replicating plasmids or viruses. Alternatively, the expression vectors, or portions thereof, can be integrated into chromosomes of the target cells by conventional techniques such as site-specific recombination or selection of stable cell lines. In stable cell lines, at least the expression cassette portion of the expression vector is integrated into a chromosome of the target cells.

The vector construct can be designed to be suitable for expression in various target cells, including but not limited to bacteria, yeast cells, plant cells, nematode cells, insect cells, and mammalian and human cells. Methods for preparing expression vectors designed for expression of gene products in different target cells are well known in the art.

Migrastatin Analogs

Migrastatin (1) is an inhibitor of cell migration. Nakae et al., *J. Antibiot.* **2000**, *53*, 1130; Nakae et al., *J. Antibiot.* **2000**, *53*, 1228; Takemoto et al., *J. Antibiot.* **2001**, *54*, 1104; Nakamura et al., *J. Antibiot.* **2002**, *55*, 442; Woo et al. *J. Antibiot.* **2002**, *55*, 141. The structure of migrastatin is provided below.



1

According to the invention, analogs of migration bind to fascin and inhibit the activity of fascin.

Migrastatin is a macrolide natural product first isolated from a cultured broth of Streptomyces and its structure features a 14-membered macrolactone ring (FIG. 1A) (Nakae et al. 2000, Woo et al. 2002). At high micromolar concentrations, the natural product inhibits the migration of several types of tumor cells in vitro but has no effect on the biosyntheses of DNA, RNA, and protein in these cells (Nakae et al. 2000).

Two synthetic migrastatin analogs, a core macroketone and a core macrolactam (FIG. 1A), were tested for inhibition of mouse breast tumor metastasis in a mouse model (Shan et al. 2005). These two compounds are potent inhibitors of mouse breast tumor metastasis, reducing 91-99% of tumor spreading to the lung. It has been determined that the cellular basis for this effect is the interference of the formation of lamellipodia that, in turn, inhibits migration of breast tumor cells. It has been further determined that the compounds of the invention exert this effect by interacting with and inhibiting fascin.

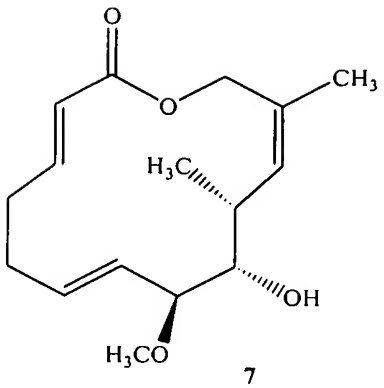
The following definitions are used, unless otherwise described: halo is fluoro, chloro, bromo, or iodo. Alkyl, alkoxy, alkenyl, alkynyl, etc. denote both straight and branched groups.

It will be appreciated by those skilled in the art that compounds of the invention having a chiral center may exist in and be isolated in optically active and racemic forms. Some compounds may exhibit polymorphism. It is to be understood that the present invention encompasses any racemic, optically-active, polymorphic, or stereoisomeric form, or mixtures thereof, of a compound of the invention, which possess the useful properties described herein, it being well known in the art how to prepare optically active forms (for example, by resolution of the racemic form by recrystallization techniques, by synthesis from optically-active starting materials, by chiral synthesis, or by chromatographic separation using a chiral stationary phase) and how to determine the cell migration inhibitory activity of such forms using the standard tests described herein, or using other similar tests which are well known in the art.

Specific and preferred values listed below for radicals, substituents, and ranges, are for illustration only; they do not exclude other defined values or other values within defined ranges for the radicals and substituents.

Specifically, (C_1-C_6)alkyl can be methyl, ethyl, propyl, isopropyl, butyl, iso-butyl, sec-butyl, pentyl, 3-pentyl, or hexyl; (C_3-C_6)cycloalkyl can be cyclopropyl, cyclobutyl, cyclopentyl, or cyclohexyl; (C_3-C_6)cycloalkyl(C_1-C_6)alkyl can be cyclopropylmethyl, cyclobutylmethyl, cyclopentylmethyl, cyclohexylmethyl, 2-cyclopropylethyl, 2-cyclobutylethyl, 2-cyclopentylethyl, or 2-cyclohexylethyl; (C_1-C_6)alkoxy can be methoxy, ethoxy, propoxy, isopropoxy, butoxy, iso-butoxy, sec-butoxy, pentoxy, 3-pentoxy, or hexyloxy.

In some embodiments, the compounds of formula I have the following structures, or pharmaceutically acceptable salts thereof.



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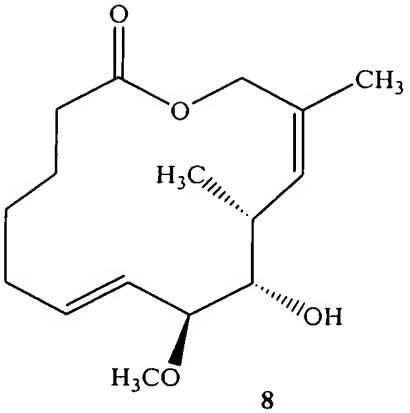

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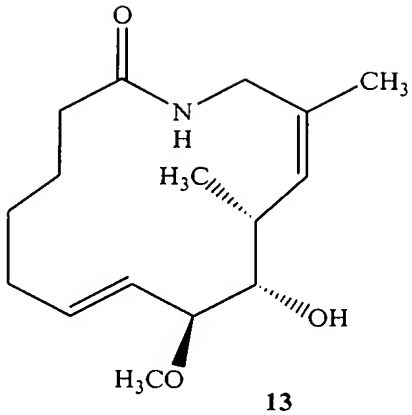

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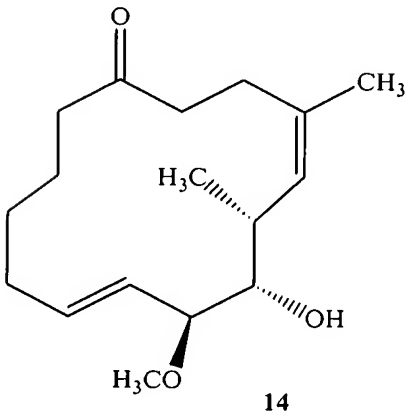

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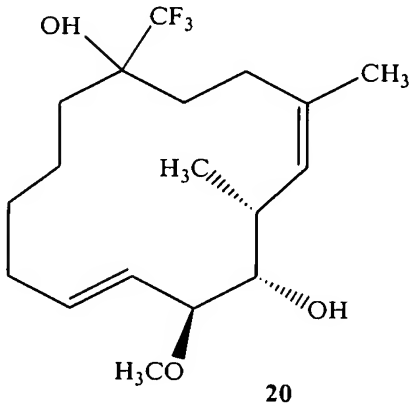

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Procedures available in the art can be used for synthesizing the compounds of the invention. For example, the compounds of the invention can be made as described in Njardarson et al., J. Am. Chem. Soc. 2004, 126, 1038-1040.

Further details on synthesizing organic compounds can be found in the art, for example, in Greene, T.W.; Wutz, P.G.M. "Protecting Groups In Organic

Synthesis" second edition, 1991, New York, John Wiley & sons, Inc. The Examples provided herein further illustrate synthetic procedures for the compounds of formula I.

In cases where compounds (e.g., the migrastatin analogs and inhibitory nucleic acids described herein) are sufficiently basic or acidic to form stable nontoxic acid or base salts, administration of the compounds as salts may be appropriate. Certain of the compounds of present invention can exist in free form for treatment, or where appropriate, as a pharmaceutically acceptable derivative thereof. According to the present invention, a pharmaceutically acceptable derivative includes, but is not limited to, pharmaceutically acceptable salts, esters, salts of such esters, or a prodrug or other adduct or derivative of a compound of this invention which upon administration to a patient in need is capable of providing, directly or indirectly, a compound as otherwise described herein, or a metabolite or residue thereof.

As used herein, the term "pharmaceutically acceptable salt" refers to those salts which are, within the scope of sound medical judgment, suitable for use in contact with the tissues of humans and lower animals without undue toxicity, irritation, allergic response and the like, and are commensurate with a reasonable benefit/risk ratio. Pharmaceutically acceptable salts of amines, carboxylic acids, and other types of compounds, are well known in the art. For example, S. M. Berge, et al. describe pharmaceutically acceptable salts in detail in J Pharmaceutical Sciences, 66: 1-19 (1977), incorporated herein by reference. The salts can be prepared in situ during the final isolation and purification of the compounds of the invention, or separately by reacting a free base or free acid function with a suitable reagent. For example, a free base function can be reacted with a suitable acid.

Furthermore, where the compounds of the invention carry an acidic moiety, suitable pharmaceutically acceptable salts thereof may, include metal salts such as alkali metal salts, e. g. sodium or potassium salts; and alkaline earth metal salts, e. g. calcium or magnesium salts. Examples of pharmaceutically acceptable, nontoxic acid addition salts are salts of an amino group formed with inorganic acids such as hydrochloric acid, hydrobromic acid, phosphoric acid, sulfuric acid and perchloric

acid or with organic acids such as acetic acid, oxalic acid, maleic acid, tartaric acid, citric acid, succinic acid or malonic acid or by using other methods used in the art such as ion exchange. Other pharmaceutically acceptable salts include adipate, alginate, ascorbate, aspartate, benzenesulfonate, benzoate, bisulfate, borate, butyrate, camphorate, camphorsulfonate, citrate, cyclopentanepropionate, digluconate, dodecylsulfate, ethanesulfonate, formate, fumarate, glucoheptonate, glycerophosphate, gluconate, hemisulfate, heptanoate, hexanoate, hydroiodide, 2-hydroxy-ethanesulfonate, lactobionate, lactate, laurate, lauryl sulfate, malate, maleate, malonate, methanesulfonate, 2-naphthalenesulfonate, nicotinate, nitrate, oleate, oxalate, palmitate, pamoate, pectinate, persulfate, 3-phenylpropionate, phosphate, picrate, pivalate, propionate, stearate, succinate, sulfate, tartrate, thiocyanate, p- toluenesulfonate, undecanoate, valerate salts, and the like. Representative alkali or alkaline earth metal salts include sodium, lithium, potassium, calcium, magnesium, and the like. Further pharmaceutically acceptable salts include, when appropriate, nontoxic ammonium, quaternary ammonium, and amine cations formed using counterions such as halide, hydroxide, carboxylate, sulfate, phosphate, nitrate, lower alkyl sulfonate and aryl sulfonate.

Pharmaceutically acceptable salts may be obtained using standard procedures well known in the art, for example, by reacting a sufficiently basic compound such as an amine with a suitable acid affording a physiologically acceptable anion. Alkali metal (for example, sodium, potassium or lithium) or alkaline earth metal (for example calcium) salts of carboxylic acids can also be made.

Additionally, as used herein, the term "pharmaceutically acceptable ester" refers to esters that hydrolyze in vivo and include those that break down readily in the human body to leave the parent compound or a salt thereof. Suitable ester groups include, for example, those derived from pharmaceutically acceptable aliphatic carboxylic acids, particularly alkanoic, alkenoic, cycloalkanoic and alkanedioic acids, in which each alkyl or alkenyl moiety advantageously has not more than 6 carbon atoms. Examples of particular esters include formates, acetates, propionates, butyrates, acrylates and ethylsuccinates.

Furthermore, the term "pharmaceutically acceptable prodrugs" as used herein refers to those prodrugs of the compounds of the present invention which are, within the scope of sound medical judgment, suitable for use in contact with the tissues of humans and other mammals with undue toxicity, irritation, allergic response, and the like, commensurate with a reasonable benefit/risk ratio, and effective for their intended use, as well as the zwitterionic forms, where possible, of the compounds of the invention. The term "prodrug" refers to compounds that are rapidly transformed in vivo to yield the parent compound of formula I described herein, for example by hydrolysis in blood. A thorough discussion is provided in T. Higuchi and V. Stella, Pro-drugs as Novel Delivery Systems, Vol. 14 of the A.C.S. Symposium Series, and in Edward B. Roche, ed. , Bioreversible Carriers in Drug Design, American Pharmaceutical Association and Pergamon Press, 1987, both of which are incorporated herein by reference.

Anti-Fascin Antibodies

The invention provides antibody preparations directed against fascin, for example, antibodies capable of binding a polypeptide having SEQ ID NO:1, 3, 5, 7, 9, 10 and/or 12. In some embodiments, the antibody can bind to the actin binding sites or the migrastatin-analog binding site. For example, in some embodiments, the antibodies of the invention can bind to an epitopal site that includes any of fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473, which form key portions of the migrastatin analog binding site. In other embodiments, the antibodies of the invention can bind to an epitopal site that includes any of fascin amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250, which form key parts of one of the fascin actin binding sites.

Such antibodies are desirable to block the activity of fascin, which, as illustrated herein, is associated with metastatic cancer and tumors. Thus, antibody

preparations of the invention can serve as inhibitors of fascin activity and therefore act as therapeutic agents.

Methods are provided to prepare and screen for antibodies that preferentially recognize fascin, the fascin-actin binding sites and/or the fascin-migrastatin analog binding site. A peptide sequence that includes fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473 (the migrastatin analog binding site) and/or fascin amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250 (one of the actin binding sites) is used as antigen to raise polyclonal or monoclonal antibodies. Fascin peptides that are used to generate antibodies of the invention include peptides with the above-identified epitopal sites. For example, such fascin peptides include any peptide with a sequence that includes amino acids 259 through 493 of SEQ ID NO:1, 3, 5, 7, 9, 10 and/or 12.

The resultant antibodies are selected for binding to fascin or a selected peptide sequence (e.g., the antigenic peptide used to generate the antibodies). The antibodies can then be screened for inhibition of fascin. Inhibitory antibodies are selected by screening the antibodies for inhibition as described herein, for example, as described below and in the Examples.

Antibody molecules belong to a family of plasma proteins called immunoglobulins, whose basic building block, the immunoglobulin fold or domain, is used in various forms in many molecules of the immune system and other biological recognition systems. A typical immunoglobulin has four polypeptide chains, containing an antigen binding region known as a variable region and a non-varying region known as the constant region.

Native antibodies and immunoglobulins are usually heterotetrameric glycoproteins of about 150,000 daltons, composed of two identical light (L) chains and two identical heavy (H) chains. Each light chain is linked to a heavy chain by one covalent disulfide bond, while the number of disulfide linkages varies between the heavy chains of different immunoglobulin isotypes. Each heavy and light chain

also has regularly spaced intrachain disulfide bridges. Each heavy chain has at one end a variable domain (VH) followed by a number of constant domains. Each light chain has a variable domain at one end (VL) and a constant domain at its other end. The constant domain of the light chain is aligned with the first constant domain of the heavy chain, and the light chain variable domain is aligned with the variable domain of the heavy chain. Particular amino acid residues are believed to form an interface between the light and heavy chain variable domains (Clothia et al., J. Mol. Biol. 186, 651-66, 1985); Novotny and Haber, Proc. Natl. Acad. Sci. USA 82, 4592-4596 (1985).

Depending on the amino acid sequences of the constant domain of their heavy chains, immunoglobulins can be assigned to different classes. There are at least five (5) major classes of immunoglobulins: IgA, IgD, IgE, IgG and IgM, and several of these may be further divided into subclasses (isotypes), e.g. IgG-1, IgG-2, IgG-3 and IgG-4; IgA-1 and IgA-2. The heavy chains constant domains that correspond to the different classes of immunoglobulins are called alpha (α), delta (δ), epsilon (ε), gamma (γ) and mu (μ), respectively. The light chains of antibodies can be assigned to one of two clearly distinct types, called kappa (κ) and lambda (λ), based on the amino sequences of their constant domain. The subunit structures and three-dimensional configurations of different classes of immunoglobulins are well known.

The term "variable" in the context of variable domain of antibodies, refers to the fact that certain portions of the variable domains differ extensively in sequence among antibodies. The variable domains are for binding and determine the specificity of each particular antibody for its particular antigen. However, the variability is not evenly distributed through the variable domains of antibodies. It is concentrated in three segments called complementarity determining regions (CDRs) also known as hypervariable regions both in the light chain and the heavy chain variable domains.

The more highly conserved portions of variable domains are called the framework (FR). The variable domains of native heavy and light chains each comprise four FR regions, largely adopting a β-sheet configuration, connected by

three complementarity-determining regions (CDRs), which form loops connecting, and in some cases forming part of, the β-sheet structure. The CDRs in each chain are held together in close proximity by the FR regions and, with the CDRs from the other chain, contribute to the formation of the antigen-binding site of antibodies. The constant domains are not involved directly in binding an antibody to an antigen, but exhibit various effector functions, such as participation of the antibody in antibody-dependent cellular toxicity.

An antibody that is contemplated for use in the present invention thus can be in any of a variety of forms, including a whole immunoglobulin, an antibody fragment such as Fv, Fab, and similar fragments, a single chain antibody which includes the variable domain complementarity determining regions (CDR), and the like forms, all of which fall under the broad term "antibody", as used herein. The present invention contemplates the use of any specificity of an antibody, polyclonal or monoclonal, and is not limited to antibodies that recognize and immunoreact with a specific antigen. In preferred embodiments, in the context of both the therapeutic and screening methods described below, an antibody or fragment thereof is used that is immunospecific for an antigen or epitope of the invention.

The term "antibody" also refers to a portion of a full-length antibody, generally the antigen binding or variable region. Examples of antibody fragments that can serve as antibodies of the invention include Fab, Fab', $F(ab')_2$ and Fv fragments. Papain digestion of antibodies produces two identical antigen binding fragments, called the Fab fragment, each with a single antigen binding site, and a residual "Fc" fragment, so-called for its ability to crystallize readily. Pepsin treatment yields an $F(ab')_2$ fragment that has two antigen binding fragments that are capable of cross-linking antigen, and a residual other fragment (which is termed pFc'). Additional fragments that are included in the invention are diabodies, linear antibodies, single-chain antibody molecules, and multispecific antibodies formed from antibody fragments. In some embodiments, the antibodies are Fv, F(ab) and $F(ab')_2$ fragments.

Therefore, the antibodies contemplated by the invention therefore do not have to be full-length antibodies, so long as they bind fascin with specificity.

Moreover, the antibodies of the invention can include polypeptides having fascin binding domains, for example, fascin-binding complementarity-determining regions (CDRs). Such CDRs can be as small as about 4 amino acids, 5 amino acids, 6 amino acids, 7 amino acids, 9 amino acids, about 12 amino acids, about 15 amino acids, about 17 amino acids, about 18 amino acids, about 20 amino acids, about 25 amino acids, about 30 amino acids or more. In general, an antibody of the invention has any upper size limit so long as it binds with specificity to fascin, e.g. a polypeptide having SEQ ID NO:1, 3, 5, 7, 9, 10 and/or 12.

Antibody fragments retaining an ability to selectively bind with its antigen. Some types of antibody fragments are defined as follows:

(1) Fab is the fragment that contains a monovalent antigen-binding fragment of an antibody molecule. A Fab fragment can be produced by digestion of whole antibody with the enzyme papain to yield an intact light chain and a portion of one heavy chain.

(2) Fab' is the fragment of an antibody molecule can be obtained by treating whole antibody with pepsin, followed by reduction, to yield an intact light chain and a portion of the heavy chain. Two Fab' fragments are obtained per antibody molecule. Fab' fragments differ from Fab fragments by the addition of a few residues at the carboxyl terminus of the heavy chain CH1 domain including one or more cysteines from the antibody hinge region.

(3) $(Fab')_2$ is the fragment of an antibody that can be obtained by treating whole antibody with the enzyme pepsin without subsequent reduction. $F(ab')_2$ is a dimer of two Fab' fragments held together by two disulfide bonds.

(4) Fv is the minimum antibody fragment that contains a complete antigen recognition and binding site. This region consists of a dimer of one heavy and one light chain variable domain in a tight, non-covalent association (V_H -V_L dimer). It is in this configuration that the three CDRs of each variable domain interact to define an antigen binding site on the surface of the V_H -V_L dimer. Collectively, the six CDRs confer antigen binding specificity to the antibody. However, even a single variable domain (or half of an Fv including only three

CDRs specific for an antigen) has the ability to recognize and bind antigen, although at a lower affinity than the entire binding site.

(5) Single chain antibody ("SCA"), defined as a genetically engineered molecule containing the variable region of the light chain, the variable region of the heavy chain, linked by a suitable polypeptide linker as a genetically fused single chain molecule. Such single chain antibodies are also referred to as "single-chain Fv" or "sFv" antibody fragments. Generally, the Fv polypeptide further includes a polypeptide linker between the VH and VL domains that enables the sFv to form the desired structure for antigen binding. For a review of sFv see Pluckthun in The Pharmacology of Monoclonal Antibodies, vol. 113, Rosenburg and Moore eds. Springer-Verlag, N.Y., pp. 269-315 (1994).

The term "diabodies" refers to a small antibody fragments with two antigen-binding sites, which fragments comprise a heavy chain variable domain (VH) connected to a light chain variable domain (VL) in the same polypeptide chain (VH-VL). By using a linker that is too short to allow pairing between the two domains on the same chain, the domains are forced to pair with the complementary domains of another chain and create two antigen-binding sites. Diabodies are described more fully in, for example, EP 404,097; WO 93/11161, and Hollinger et al., Proc. Natl. Acad Sci. USA 90: 6444-6448 (1993).

Methods for preparing polyclonal antibodies are available to those skilled in the art. See, for example, Green, et al., Production of Polyclonal Antisera, in: Immunochemical Protocols (Manson, ed.), pages 1-5 (Humana Press); Coligan, et al., Production of Polyclonal Antisera in Rabbits, Rats Mice and Hamsters, in: Current Protocols in Immunology, section 2.4.1 (1992), which are hereby incorporated by reference.

Methods for preparing monoclonal antibodies are likewise available to one of skill in the art. See, for example, Kohler & Milstein, Nature, 256:495 (1975); Coligan, et al., sections 2.5.1-2.6.7; and Harlow, et al., in: Antibodies: A Laboratory Manual, page 726 (Cold Spring Harbor Pub. (1988)), which are hereby incorporated by reference. Monoclonal antibodies can be isolated and purified from hybridoma cultures by a variety of well-established techniques. Such isolation

techniques include affinity chromatography with Protein-A Sepharose, size-exclusion chromatography, and ion-exchange chromatography. See, e.g., Coligan, et al., sections 2.7.1-2.7.12 and sections 2.9.1-2.9.3; Barnes, et al., Purification of Immunoglobulin G (IgG), in: Methods in Molecular Biology, Vol. 10, pages 79-104 (Humana Press (1992).

Methods of *in vitro* and *in vivo* manipulation of monoclonal antibodies are also available to those skilled in the art. For example, monoclonal antibodies to be used in accordance with the present invention may be made by the hybridoma method first described by Kohler and Milstein, Nature 256, 495 (1975), or may be made by recombinant methods, e.g., as described in U.S. Pat. No. 4,816,567. The monoclonal antibodies for use with the present invention may also be isolated from phage antibody libraries using the techniques described in Clackson et al. Nature 352: 624-628 (1991), as well as in Marks et al., J. Mol Biol. 222: 581-597 (1991). Another method involves humanizing a monoclonal antibody by recombinant means to generate antibodies containing human specific and recognizable sequences. See, for review, Holmes, et al., J. Immunol., 158:2192-2201 (1997) and Vaswani, et al., Annals Allergy, Asthma & Immunol., 81:105-115 (1998).

The term "monoclonal antibody" as used herein refers to an antibody obtained from a population of substantially homogeneous antibodies, i.e., the individual antibodies comprising the population are identical except for possible naturally occurring mutations that may be present in minor amounts. Monoclonal antibodies are highly specific, being directed against a single antigenic site. Furthermore, in contrast to conventional polyclonal antibody preparations that typically include different antibodies directed against different determinants (epitopes), each monoclonal antibody is directed against a single determinant on the antigen. In additional to their specificity, the monoclonal antibodies are advantageous in that they are synthesized by the hybridoma culture, uncontaminated by other immunoglobulins. The modifier "monoclonal" indicates that the antibody preparation is a substantially homogeneous population of antibodies, and is not to be construed as requiring production of the antibody by any particular method.

The monoclonal antibodies herein specifically include "chimeric" antibodies (immunoglobulins) in which a portion of the heavy and/or light chain is identical with or homologous to corresponding sequences in antibodies derived from a particular species or belonging to a particular antibody class or subclass, while the remainder of the chain(s) is identical with or homologous to corresponding sequences in antibodies derived from another species or belonging to another antibody class or subclass, as well as fragments of such antibodies, so long as they exhibit the desired biological activity (U.S. Pat. No. 4,816,567); Morrison et al. Proc. Natl. Acad Sci. 81, 6851-6855 (1984).

Methods of making antibody fragments are also known in the art (see for example, Harlow and Lane, Antibodies: A Laboratory Manual, Cold Spring Harbor Laboratory, New York, (1988), incorporated herein by reference). Antibody fragments of the present invention can be prepared by proteolytic hydrolysis of the antibody or by expression in *E. coli* of DNA encoding the fragment. Antibody fragments can be obtained by pepsin or papain digestion of whole antibodies conventional methods. For example, antibody fragments can be produced by enzymatic cleavage of antibodies with pepsin to provide a 5S fragment denoted $F(ab')_2$. This fragment can be further cleaved using a thiol reducing agent, and optionally a blocking group for the sulfhydryl groups resulting from cleavage of disulfide linkages, to produce 3.5S Fab' monovalent fragments. Alternatively, an enzymatic cleavage using pepsin produces two monovalent Fab' fragments and an Fc fragment directly. These methods are described, for example, in U.S. Patents No. 4,036,945 and No. 4,331,647, and references contained therein. These patents are hereby incorporated in their entireties by reference.

Other methods of cleaving antibodies, such as separation of heavy chains to form monovalent light-heavy chain fragments, further cleavage of fragments, or other enzymatic, chemical, or genetic techniques may also be used, so long as the fragments bind to the antigen that is recognized by the intact antibody. For example, Fv fragments comprise an association of V_H and V_L chains. This association may be non-covalent or the variable chains can be linked by an intermolecular disulfide bond or cross-linked by chemicals such as glutaraldehyde.

Preferably, the Fv fragments comprise V_H and V_L chains connected by a peptide linker. These single-chain antigen binding proteins (sFv) are prepared by constructing a structural gene comprising DNA sequences encoding the V_H and V_L domains connected by an oligonucleotide. The structural gene is inserted into an expression vector, which is subsequently introduced into a host cell such as *E. coli*. The recombinant host cells synthesize a single polypeptide chain with a linker peptide bridging the two V domains. Methods for producing sFvs are described, for example, by Whitlow, et al., Methods: a Companion to Methods in Enzymology, Vol. 2, page 97 (1991); Bird, et al., Science 242:423-426 (1988); Ladner, et al, US Patent No. 4,946,778; and Pack, et al., Bio/Technology 11:1271-77 (1993).

Another form of an antibody fragment is a peptide coding for a single complementarity-determining region (CDR). CDR peptides ("minimal recognition units") are often involved in antigen recognition and binding. CDR peptides can be obtained by cloning or constructing genes encoding the CDR of an antibody of interest. Such genes are prepared, for example, by using the polymerase chain reaction to synthesize the variable region from RNA of antibody-producing cells. See, for example, Larrick, et al., Methods: a Companion to Methods in Enzymology, Vol. 2, page 106 (1991).

The invention contemplates human and humanized forms of non-human (e.g. murine) antibodies. Such humanized antibodies are chimeric immunoglobulins, immunoglobulin chains or fragments thereof (such as Fv, Fab, Fab', $F(ab')_2$ or other antigen-binding subsequences of antibodies) that contain minimal sequence derived from non-human immunoglobulin. For example, humanized antibodies can be made from a human immunoglobulins (recipient antibody) in which residues from a complementary determining region (CDR) of the recipient are replaced by residues from a CDR of a nonhuman species (donor antibody) such as mouse, rat or rabbit having the desired specificity, affinity and capacity.

In some instances, Fv framework residues of the human immunoglobulin are replaced by corresponding non-human residues. Furthermore, humanized antibodies may comprise residues that are found neither in the recipient antibody nor in the

imported CDR or framework sequences. These modifications are made to further refine and optimize antibody performance. In general, humanized antibodies will comprise substantially all of at least one, and typically two, variable domains, in which all or substantially all of the CDR regions correspond to those of a non-human immunoglobulin and all or substantially all of the FR regions are those of a human immunoglobulin consensus sequence. The humanized antibody optimally also will comprise at least a portion of an immunoglobulin constant region (Fc), typically that of a human immunoglobulin. For further details, see: Jones et al., Nature 321, 522-525 (1986); Reichmann et al., Nature 332, 323-329 (1988); Presta, Curr. Op. Struct. Biol. 2, 593-596 (1992); Holmes, et al., J. Immunol., 158:2192-2201 (1997) and Vaswani, et al., Annals Allergy, Asthma & Immunol., 81:105-115 (1998).

The invention also provides methods of mutating antibodies to optimize their affinity, selectivity, binding strength or other desirable property. A mutant antibody refers to an amino acid sequence variant of an antibody. In general, one or more of the amino acid residues in the mutant antibody is different from what is present in the reference antibody. Such mutant antibodies necessarily have less than 100% sequence identity or similarity with the reference amino acid sequence. In general, mutant antibodies have at least 75% amino acid sequence identity or similarity with the amino acid sequence of either the heavy or light chain variable domain of the reference antibody. Preferably, mutant antibodies have at least 80%, more preferably at least 85%, even more preferably at least 90%, and most preferably at least 95% amino acid sequence identity or similarity with the amino acid sequence of either the heavy or light chain variable domain of the reference antibody. One method of mutating antibodies involves affinity maturation using phage display.

The invention is therefore directed to a method for selecting antibodies and/or antibody fragments or antibody polypeptides with desirable properties. Such desirable properties can include increased binding affinity or selectivity for fascin and/or fascin epitopes (e.g., the fascin actin or migrastatin binding sites of the invention).

The antibodies and antibody fragments of the invention are isolated antibodies and antibody fragments. An isolated antibody is one that has been identified and separated and/or recovered from a component of the environment in which it was produced. Contaminant components of its production environment are materials that would interfere with diagnostic or therapeutic uses for the antibody, and may include antigenic proteins, enzymes, hormones, and other proteinaceous or nonproteinaceous solutes. The term "isolated antibody" also includes antibodies within recombinant cells because at least one component of the antibody's natural environment will not be present. In some embodiments, however, an isolated antibody will be at least partially purified, for example, by employing at least one purification step.

If desired, the antibodies of the invention can be purified by any available procedure. For example, the antibodies can be affinity purified by binding an antibody preparation to a solid support to which the antigen used to raise the antibodies is bound. After washing off contaminants, the antibody can be eluted by known procedures. Those of skill in the art will know of various techniques common in the immunology arts for purification and/or concentration of polyclonal antibodies, as well as monoclonal antibodies (see for example, Coligan, et al., Unit 9, Current Protocols in Immunology, Wiley Interscience, 1991, incorporated by reference).

In some embodiments, the antibody will be purified as measurable by at least three different methods: 1) to greater than 95% by weight of antibody as determined by the Lowry method, and most preferably more than 99% by weight; 2) to a degree sufficient to obtain at least 15 residues of N-terminal or internal amino acid sequence by use of a spinning cup sequentator; or 3) to homogeneity by SDS-PAGE under reducing or non-reducing conditions using Coomasie blue or, preferably, silver stain.

Fascin Structure

The invention further relates to the three dimensional structure of fascin. Table 2 provides the three-dimensional coordinates for the atoms in fascin. As

described in more detail in Example 9, fascin has two actin binding sites. When fascin binds to actin it facilitates formation of actin bundles. For example, addition of fascin induced the formation of F-actin bundles (FIG. 6B).

One of the primary actin binding sites of fascin is the binding site for migrastatin analogs. The second actin binding site includes fascin amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250.

Migrastatin analogs can bind to at least one of the actin binding sites and such binding inhibits actin bundling. For example, the migrastatin analog, macroketone, binds at the surface of trefoil 4, on the side facing the cleft between trefoil 4 and trefoil 1 (FIG. 10C). Macroketone is held in place by interacting with the side chains of His392, Glu391, Ala488, Lys471, and His474 as well as the alpha carbon of Asp473 (FIG. 11 A–D). The six residues form a U-shape curvature, holding macroketone like holding a ring with thumb and index finger (FIG. 11A and 11B). On the top of the two "fingers" are the two histidines, His392 and His474, which have major contributions to the fascin-macroketone interaction. The NE2 nitrogen of His392 is 3.01 Å away from the ketone oxygen of macroketone molecule, while the ND1 nitrogen of His474 is 2.57 Å away from the hydroxyl oxygen. His392 and His474 contribute to the binding of macroketone by forming hydrogen bonds with macroketone (FIG. 11B). The interaction between fascin and macroketone is further stabilized by the *van der Waals* force between the macrolide ring carbon and residue Glu391, Ala488, Lys471 and Asp473 (FIG. 11B).

While addition of fascin induced the formation of F-actin bundles (FIG. 6B), in the presence of macroketone, formation of F-actin bundles was largely (>80%) inhibited (FIG. 6B and 6C).

As described herein, fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473 form portions of the migrastatin analog binding site.

Thus, as described herein, fascin has two binding sites. Actin can interact with both sites. However, the migrastatin analogs apparently interact with only one

site. The migrastatin analog binding site is a U-shaped cleft or pocket with dimensions of about eight (8) by ten (10) by ten (10) angstroms (i.e., 8Å x 10Å x 10Å). The other binding site for actin on fascin is also U-shaped, but it runs along the surface of fascin and is not an indented pocket.

Methods of Detecting and Isolating Agents that can Modulate Fascin

The invention further provides screening methods and assays that are useful for generating or identifying therapeutic agents for inhibiting fascin and the diseases associated with fascin activity.

One skilled in the art may use one of several methods to screen test agents for their ability to associate, bind and/or modulate the activity of fascin. For example, one of skill in the art may use the fascin structure described herein to identify the type, shape and structure of molecules that can interact with fascin actin and migrastatin analog binding sites. One of skill in the art may also screen test agents by observing whether a test agent binds to fascin and/or inhibits cell migration. These methods are described in more detail below.

Binding sites, also referred to as binding pockets in the present invention, are of significant utility in fields such as drug discovery. Such binding pockets or sites are the locus of fascin's actin bundling activity. Moreover, identification of the location and composition of the actin and migrastatin analog binding sites facilitates discovery of small molecules, drugs and or factors that interact with, bind and/or modulate fascin activity. An understanding of the size, structure and composition of fascin-actin and fascin-migrastatin analog binding sites also facilitates the design of drugs having more favorable associations with these binding sites, and thus, provides drugs and therapeutic agents with improved biological effects. For example, the fascin three dimensional structure and the physical and chemical properties of the fascin binding sites facilitates design of inhibitors that interact with, bind or block those binding sites.

Test agents that exhibit an appropriate size, atomic structure and chemical make-up may be tested further in actual binding assays, cell migration assays and the like to ascertain whether those test agents are viable candidates for development

as therapeutic agents for inhibiting fascin in vivo. This screening process may begin by visual inspection of, for example, one of the actin or migrastatin analog binding sites on the computer screen using the fascin three dimensional atomic coordinates in Table 2 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical moieties may then be positioned in a variety of orientations, or docked, within that binding site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical moieties. These include: 1. GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK. 2. MCSS (A. Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, San Diego, Calif. 3. AUTODOCK (D. S. Goodsell et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, 8, pp. 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, Calif. 4. DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable chemical entities or moieties have been selected, they can be assembled into a single test agent (e.g., a compound or complex). Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of fascin. This would be followed by manual model building using software such as Quanta or Sybyl [Tripos Associates, St. Louis, Mo.].

Useful programs to aid one of skill in the art in selecting and joining the individual chemical moieties or fragments include: 1. CAVEAT (P. A. Bartlett et al,

"CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989); G. Lauri and P. A. Bartlett, "CAVEAT: a Program to Facilitate the Design of Organic Molecules", J. Comput. Aided Mol. Des., 8, pp. 51-66 (1994)). CAVEAT is available from the University of California, Berkeley, Calif. 2. 3D Database systems such as ISIS (MDL Information Systems, San Leandro, Calif.). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992). 3 HOOK (M. B. Eisen et al, "HOOK: A Program for Finding Novel Molecular Architectures that Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site", Proteins: Struct., Funct., Genet., 19, pp. 199-221 (1994). HOOK is available from Molecular Simulations, San Diego, Calif.

Instead of proceeding to build an modulator or inhibitor of fascin in a step-wise fashion by defining one moiety or chemical fragment at a time as described above, test agents that can bind fascin can be designed as a whole or "de novo" using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). There are many de novo ligand design methods including: 1. LUDI (H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Molecular Simulations Incorporated, San Diego, Calif. 2. LEGEND (Y. Nishibata et al., Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations Incorporated, San Diego, Calif. 3. LeapFrog (available from Tripos Associates, St. Louis, Mo.). 4. SPROUT (V. Gillet et al, "SPROUT: A Program for Structure Generation)", J. Comput. Aided Mol. Design, 7, pp. 127-153 (1993)). SPROUT is available from the University of Leeds, UK.

Other molecular modeling techniques may also be employed in accordance with this invention [see, e.g., N. C Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990); see also, M. A. Navia and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992); L. M.

Balbes et al., "A Perspective of Modern Methods in Computer-Aided Drug Design", in Reviews in Computational Chemistry, Vol. 5, K. B. Lipkowitz and D. B. Boyd, Eds., VCH, New York, pp 337-380 (1994); see also, W. C. Guida, "Software For Structure-Based Drug Design", Curr. Opin. Struct. Biology, 4, pp. 777-781 (1994)].

Once a test agent has been designed or selected by the above methods, the efficiency with which that test agent binds to a fascin binding site can be tested and optimized by computational evaluation. For example, an effective fascin binding site inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient fascin binding site inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. Fascin binding site inhibitors may interact with the binding site in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

A test agent designed or selected as binding to a fascin binding site may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target binding site and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Thus, the chemical composition and positions of charged, hydrophilic, and hydrophobic moieties within the fascin binding sites can be evaluated and compared to those of the test agent. As described above, the primary actin binding site of fascin include fascin amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250. Moreover, fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473 form portions of the migrastatin analog binding site.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Thus, for example, the test agents can be evaluated using such programs as: Gaussian 94, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa., 1995); AMBER, version 4.1 (P. A. Kollman, University of California at San Francisco, 1995); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, Calif. 01995); Insight II/Discover (Molecular Simulations, Inc, San Diego, Calif. .COPYRGT.1995); DelPhi (Molecular Simulations, Inc., San Diego, Calif. 1995); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach is the computational screening of small molecule databases for test agents that can bind in whole, or in part, to a fascin binding site. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy [E. C. Meng et al., J. Comp. Chem., 13, pp. 505-524 (1992)].

Therefore, one aspect of this invention is a machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when used by a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex comprising a binding site defined by structure coordinates of fascin amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250 (actin binding site) according to Table 2, or a homolog of said molecule or molecular complex, wherein said homolog comprises a binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms.

Another aspect of the invention, is a machine-readable data storage medium, comprising a data storage material encoded with machine readable data which,

when used by a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex comprising a binding site defined by structure coordinates of fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473 (portions of the migrastatin analog binding site) according to Table 2, or a homolog of said molecule or molecular complex, wherein said homolog comprises a binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms.

Preferably, the machine readable data, when used by a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex comprising a binding site defined by structure coordinates fascin amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250 (actin binding site) or by the structure coordinates of fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473 (portions of the migrastatin analog binding site) according to Table 2, or a homolog of said molecule or molecular complex, wherein said homolog comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms.

In another embodiment, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine readable data which comprises the Fourier transform of the structure coordinates set forth in Table 2, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pattern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

For example, the Fourier transform of the structure coordinates set forth in Table 2 may be used to determine at least a portion of the structure coordinates of

other fascins, such as fascin 2, fascin 3, fascin homolog 1 and isoforms of fascin 2, fascin 3, fascin homolog 1.

FIG. 15 demonstrates one version of these embodiments. System **10** includes a computer **11** comprising a central processing unit ("CPU") **20**, a working memory **22** which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory **24** (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals **26**, one or more keyboards **28**, one or more input lines **30**, and one or more output lines **40**, all of which are interconnected by a conventional bi-directional system bus **50**.

Input hardware **36**, coupled to computer **11** by input lines **30**, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems **32** connected by a telephone line or dedicated data line **34**. Alternatively or additionally, the input hardware **36** may comprise CD-ROM drives or disk drives **24**. In conjunction with display terminal **26**, keyboard **28** may also be used as an input device.

Output hardware **46**, coupled to computer **11** by output lines **40**, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal **26** for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer **42**, so that hard copy output may be produced, or a disk drive **24**, to store system output for later use.

In operation, CPU **20** coordinates the use of the various input and output devices **36**, **46**, coordinates data accesses from mass storage **24** and accesses to and from working memory **22**, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system **10** are included as appropriate throughout the following description of the data storage medium.

Another aspect of the invention is a computer for producing a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding site defined by fascin amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250 (actin binding site) or by fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473 (portions of the migrastatin analog binding site) according to Table 2, or a homolog of said molecule or molecular complex, wherein said homolog comprises a binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms, wherein said computer comprises: (a) a machine readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said machine readable data comprises the structure coordinates of fascin or portions thereof; (b) a working memory for storing instructions for processing said machine-readable data; (c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium, for processing said machine-readable data into said three-dimensional representation; and (d) an output hardware coupled to said central processing unit, for receiving said three dimensional representation.

In some embodiments, the computer produces a three-dimensional representation of a molecule or molecular complex of an actin binding site, wherein said molecule or molecular complex comprises a binding pocket defined by the structural coordinates of fascin amino acid residues Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250 (actin binding site) or by the structure coordinates of fascin amino acid residues His392, Glu391, Ala488, Lys471, His474 and Asp473 (portions of the migrastatin analog binding site) according to Table 2, or a homolog of said molecule or molecular complex, wherein said homolog comprises a binding

pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms.

In some embodiments, the structure of a fascin polypeptide fragment can used for generating such a three-dimensional representation, where the fascin polypeptide fragment includes the actin binding site and/or the migrastatin analog binding site , e.g., any of SEQ ID NO:9-12.

FIG. 16 shows a cross section of a magnetic data storage medium **100** which can be encoded with a machine-readable data that can be carried out by a system such as system **10** of FIG. 15. Medium **100** can be a conventional floppy diskette or hard disk, having a suitable substrate **101**, which may be conventional, and a suitable coating **102**, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium **100** may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device **24**.

The magnetic domains of coating **102** of medium **100** are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system **10** of FIG. 15.

FIG. 17 shows a cross section of an optically-readable data storage medium **110** which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system **10** of FIG. 15. Medium **110** can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium **100** preferably has a suitable substrate **111**, which may be conventional, and a suitable coating **112**, which may be conventional, usually of one side of substrate **111**.

In the case of CD-ROM, as is well known, coating **112** is reflective and is impressed with a plurality of pits **113** to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating **112**. A protective coating **114**, which preferably is substantially transparent, is provided on top of coating **112**.

In the case of a magneto-optical disk, as is well known, coating **112** has no pits **113**, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating **112**. The arrangement of the domains encodes the data as described above.

Thus, in accordance with the present invention, data capable of displaying the three dimensional structure of fascin and portions thereof and their structurally similar homologues is stored in a machine-readable storage medium, which is capable of displaying a graphical three-dimensional representation of the structure.

Thus, the fascin X-ray coordinate data, for example, when used in conjunction with a computer programmed with software to translate those coordinates into the 3-dimensional structure of fascin, can be used for a variety of purposes, such as drug discovery.

Methods for identifying test agents that interact with fascin, where the physical interaction is detected, are also encompassed by the invention. Test agents can be screened and likely candidates can be identified by biological assays and binding assays. Moreover, the candidate inhibitors identified using the computer assisted structural design methods described above can be further tested and screened for useful biological activities using such biological assays and binding assays.

Binding assays between fascin and test agents may be carried out in several formats, including cell-based binding assays, solution-phase assays, solid phase based assays and immunoassays. In general, test agents are incubated with fascin for a specified period of time followed by measurement of binding between the tumor-specific protease and the test sample or compound. A label or reporter molecule attached to the fascin or a test agent can be employed, which is detectable by microscopy, fluorimetry, a scintillation counter, an enzyme or any available immunoassay.

In general, an assay for identifying compounds or molecules that interact with fascin involves incubating the fascin with a test sample that may contain such a

compound or molecule under conditions that permit binding of the compound or molecule to the fascin, and measuring whether binding has occurred. Fascin may be purified or present in mixtures, such as in cultured cells, tissue samples, body fluids, culture medium or an aqueous in vitro solution. Assays can be used that are qualitative or quantitative. Quantitative assays can be used for determining the binding parameters (affinity constants and kinetics) of the test agent or candidate fascin inhibitor for fascin. Assays may also be used to evaluate the binding of a test agent to fascin fragments, fascin domains (e.g., the fascin actin binding domain or the fascin migrastatin analog binding domain).

The test agent may be substantially purified or present in a crude mixture. Test agents can be nucleic acids, proteins, peptides, carbohydrates, lipids or small molecular weight organic compounds. The test agents can be further characterized by their ability to increase or decrease fascin activity in order to determine whether they stimulate or inhibit fascin activity.

For example, fascin affinity assays can be performed where fascin is bound to a solid substrate and the bound fascin is exposed to individual test agents or mixtures of test agents. Test agents that bind to the fascin are candidate fascin modulating agents. The solid substrate can be any convenient solid surface such as a bead, microtiter well, or column matrix. Test agents can also be separately incubated with fascin and the fascin-test agent mixture electrophoretically separated under mild, non-denaturing conditions. When a test agent binds to fascin the apparent molecular weight of the fascin-test agent complex will be greater than the molecular weight of fascin alone. Such a shift in molecular weight can readily be visualized by staining the electrophoretically separated mixtures (e.g., in a polyacrylamide gel). Test agents can also be screened to ascertain whether they competitively inhibit actin binding or binding of migrastatin analogs to fascin. In such a competitive binding assay, the amount of actin bound to fascin can be quantified, for example, by observing how much labeled actin remains associated or bound to fascin after exposure and incubation with a test agent. Thus, for example, binding can be detected by labeling actin a competitive radioimmunoassay.

These and other procedures that are readily available to those of skill in the art can be employed to identify agents that can bind to fascin.

When evidence exists that a test agent can bind to fascin, that test agent can be further tested in biological assays to determine whether it can inhibit the activity of fascin. Alternatively, biological assays can be used to screen for useful fascin modulating agents. As described herein, fascin facilitates actin bundling. Thus, test agents can be screened to ascertain whether they inhibit actin bundling by fascin using, for example, the F-actin pelleting assay described herein (or that described by Yamashiro-Matsumura et al. 1985). Such an assay involves low-speed centrifugation where the actin bundles are pelleted. For example, as shown in FIG. 6A, addition of purified fascin to F-actin increased the amounts of F-actin bundles in the pellets. Test agents that inhibit such actin bundling are candidate fascin inhibitors or modulating agents.

While fascin may be involved in the prognosis of a variety of diseases, metastasis of cancer is one of the more significant diseases in which fascin plays a role. One method of screening whether test agents and/or candidate fascin inhibitors have useful anti-metastasis activity is the Boyden Chamber Cell Migration Assay, which involves an upper and a lower set of wells separated by a cell-permeable membrane. Cells (typically cancer cells) are suspended in one chamber and a chemoattractant can be present in a lower chamber. The test agent can be placed in the upper chamber or in both chambers. Cells will migrate through the membrane to the lower chamber if the test agent does not inhibit such migration (e.g., because the test agent inhibits fascin bundling of actin). The Example of this application further illustrate and describe this type of assay.

Further assays can be performed to assess the *in vivo* toxicity and *in vivo* efficacy of a test agent or drug candidate for treating disease (e.g. cancer). Suitable animal models and tumor cell lines can be used for these purposes. For example, mice, rats or other model animals with a propensity for developing cancer can be employed. Alternatively, small tumors or tumor cells or cancer cells that are known to metastasize can be transplanted into the model animals. The tumor or cancer cells can be treated with the test agent prior to transplantation. Alternatively, some of the

animals that received tumors, tumor cells or cells then treated with the test agent or candidate fascin inhibitor. Other of those animals are control animals and/or are treated with a control agent. Tumor growth and physical signs can be monitored daily including any gross evidence of tumor necrosis, local tumor ulceration as well as evidence of toxicity including mobility, response to stimulus, eating, and weight of each animal. Test agents or candidate inhibitors that effectively reduce or eliminate tumors while having minimal negative effects on the health, lifespan and tissue integrity of the model animal are selected for development as chemotherapeutic agents and/or inhibitors of metastasis.

Assays may be used to identify agents that can interact with a cancer cell of interest. A wide variety of assays may be used for this purpose. See, for example, the assays carried out within the National Cancer Institute's "*In Vitro* Cell Line Screening Project." In general, such an assay can involve contacting a cancer cell of interest with at least one agent and observing whether the agent kills the cancer cell and/or has other deleterious effects upon that cell.

Pluralities of assays can be performed in parallel with different test agents or candidate fascin inhibitors at different concentrations to obtain a differential response to the various concentrations. Typically, at least one control assay is included in the testing. Such a control can be a negative control involving exposure of the cancer cells of interest to a physiologic solution containing no agents. Another control can involve exposure of the cancer cell of interest to an agent that has already been observed to adversely affect the cancer cell of interest, or a second cell that is related to the cell of interest. Another control can involve exposing a cell of interest to a known therapeutic compound that has a desired effect on the cancer cell of interest, for example, an anti-cancer agent with known efficacy at a particular concentration or dosage. One of skill in the art can readily select control compounds and conditions that facilitate screening and analysis of the effects of the cyclic peptides on a cancer cell of interest.

Any cell type can be assayed by these methods. For example, any mammalian or other animal cancer cell type can be screened to assess whether the agents of the invention can selectively interact therewith. Mammalian or other

animal cells can also be screened to ascertain whether the agents of the invention selectively interact therewith and/or to determine whether the agents of the invention do not interact, bind, lyse, kill or otherwise adversely affect the viability of the mammalian or other animal cell.

Conditions for screening include conditions that are used by one of skill in the art to grow, maintain or otherwise culture cell types of interest. Cancer cell types of interest should be assayed under conditions where they would be healthy but for the presence of the agents. Controls can be performed where the cell types are maintained under the selected culture conditions and not exposed to an agent, to assess whether the culture conditions influenced the viability of the cells. One of skill in the art can also perform the assay on cells that have been washed in simple physiological solutions, such as buffered saline, to eliminate, or test for, any interaction between the agents or cells and the components in the culture media. However, culture conditions for the assays generally include providing the cells with the appropriate concentration of nutrients, physiological salts, buffers and other components typically used to culture or maintain cells of the selected type. A variety of other reagents may be included in the screening assay. These include reagents like salts, neutral proteins, albumin, and serum (e.g. fetal calf serum) that are used to mimic the physiologic state of the cell types of interest. Conditions and media for culturing, growing and maintaining cells are available to one of skill in the art.

The selected reagents and components are added to the assay in the order selected by one of skill in the art. In general, the agents are added last to start the assay. Assays are performed at any suitable temperature, typically between 4 °C and 40 °C. For example, the temperature may generally range from about room temperature (about 20 °C) to about 37 °C. Incubation periods are selected to ascertain the optimal range of activity, or to insure that the test agents do not adversely affect normal, non-cancerous cells. However, incubation times can be optimized to facilitate rapid high-throughput screening. Typically, incubation times are between about one minute and about five days, for example, from about 30 minutes to about 3 days.

Test agents having the desired activity *in vitro* may be tested for activity and/or lack of toxicity *in vivo*, in an appropriate animal model. Such animal models include primates as well as mice, rats, rabbits, cats, dogs, pigs, goats, cattle or horses. For example, the mouse is a convenient animal model for testing whether agents of the invention have toxic effects and/or to determine whether the agents can inhibit metastasis of a cancer cell.

One of skill in the art can readily perform *in vivo* evaluation of the agents of the invention. For toxicity testing, a series of test agents at different test dosages can be separately administered to different animals. A single dose or, a series of dosages can be administered to the animal. A test period is selected that permits assessment of the effects of the agent(s) on the animal. Such a test period can run from about one day to about several weeks or months.

The effect of a agent(s) on an animal can be determined by observing whether the agent adversely affects the behavior (e.g., lethargy, hyperactivity) and physiological state of the animal over the course of test period. The physiological state of the animal can be assessed by standard procedures. For example, during the test period one of skill in the art can draw blood and collect other bodily fluids to test, for example, for various enzymes, proteins, metabolites, and the like. One of skill in the art can also observe whether the animal has bloating, loss of appetite, diarrhea, vomiting, blood in the urine, loss of consciousness, and a variety of other physiological problems. After the test period, the animal can be sacrificed and anatomical, pathological, histological and other studies can be performed on the tissues or organs of the animal.

For example, to determine whether one or more test agents can inhibit cancer cell metastasis, mice are infected with the selected cancer and a selected test dosage of one or more test agents is administered shortly thereafter. Alternatively, the tumor cells can be treated with the test agent prior to transplantation of the cells into the mice. Mice are observed over the course of several days to several weeks to ascertain whether the agents protect the mice from metastasis of cancer cells. At the end of the test period, mice can be sacrificed and examined to ascertain whether the

agent has optimally protected the mice from metastasis and/or to determine whether any adverse side effects have occurred.

Controls are used to establish the effects of the cancer when the agent is not administered. Other controls can also be performed, for example, to determine the safety and efficacy of the present agents compared to that of known anti-cancer compounds and inhibitors of metastasis.

Methods of Use

Agents that modulate the activity of fascin can be used to treat a variety of diseases and conditions. For example, as illustrated herein, fascin promotes actin bundling and plays a key role in cell migration and metastasis of cancer cells. Hence, modulators and inhibitors of fascin can be used to treat and inhibit metastatic cancer, including the compounds, migrastatin analogs, inhibitory nucleic acids, anti-fascin antibodies, test agents and candidate fascin modulators described herein.

However, fascin also plays a role in other diseases and conditions. For example, neurite shape and trajectory is modulated by fascin. Kraft et al., *Phenotypes of Drosophila brain neurons in primary culture reveal a role for fascin in neurite shape and trajectory.* J. NEUROSCI. (2006). Fascin is also involved in neuronal degeneration. Fulga et al., *Abnormal bundling and accumulation of F-actin mediates tau-induced neuronal degeneration in vivo.* NAT CELL BIOL. 9(2):139-48 (2007). In addition, fascin plays a role in Hodgkin's disease. Pinkus et al., *Fascin, a sensitive new marker for Reed-Sternberg cells of Hodgkin's disease. Evidence for a dendritic or B cell derivation?* AM. J. PATHOL. (1997). Fascin also plays a role in processing and presenting antigens, for example, on antigen presenting cells. Mosialos et al., *Circulating human dendritic cells differentially express high levels of a 55-kd actin-bundling protein.* AM. J. PATHOL. 148(2): 593-600 (1996); Pinkus et al., *The role of follicular and interdigitating dendritic cells in HIV-related lymphoid hyperplasia: localization of fascin.* Mod Pathol. 10(5):421-27 (1997). Moreover, fascin also plays a role in ischemic injury. Meller et al., *Ubiquitin proteasome-mediated synaptic reorganization: a novel mechanism underlying rapid ischemic tolerance.* J Neurosci. 28(1):50-9 (2008).

According to the invention, agents that modulate fascin activity (e.g., the compounds, fascin polypeptide fragments, antibodies and inhibitory nucleic acid described herein) can be used for treating and inhibiting metastatic cancer, neuronal disorders, neuronal degeneration, inflammatory conditions, viral infections, bacterial infections, lymphoid hyperplasia, Hodgkin's disease, and ischemia-related tissue damage.

Tumor metastasis is the major cause of death of cancer patients (Weiss 2000, Fidler 2003). Thus, inhibition or prevention of tumor metastasis will significantly increase the survival rate of cancer patients, allow more moderate radiation or chemotherapy with less side-effects, and control the progression of solid tumors.

Tumor cell migration and invasion are critical steps in the process of tumor metastasis (Partin et al. 1989, Aznavoorian et al. 1993, Condeelis et al. 2005). For cell migration to proceed, the actin cytoskeleton must be reorganized by forming polymers and bundles to affect the dynamic changes of cell shapes (Jaffe et al. 2005, Matsudaira 1994, Otto 1994). Individual actin filaments are flexible and elongation of individual filaments per se is insufficient for membrane protrusion which is necessary for cell migration. Bundling of actin filaments provides rigidity to actin filaments for protrusion against the compressive force from the plasma membrane (Mogilner et al. 2005).

One of the critical actin-bundling proteins is fascin. Fascin is the primary actin cross-linker in filopodia, which are membrane protrusions critical for the migration and metastasis of cancer cells. Fascin is required to maximally cross-link the actin filaments into straight, compact, and rigid bundles. Elevated expressions of fascin mRNA and protein in cancer cells have been correlated with aggressive clinical course, poor prognosis and shorter survival.

According to the invention, metastatic cancer can be treated, prevented and/or inhibited by administering fascin inhibitors.

As used herein, the term "cancer" includes solid mammalian tumors as well as hematological malignancies. The terms "tumor cell(s)" and "cancer cell(s)" are used interchangeably herein.

"Solid mammalian tumors" include cancers of the head and neck, lung, mesothelioma, mediastinum, esophagus, stomach, pancreas, hepatobiliary system, small intestine, colon, colorectal, rectum, anus, kidney, urethra, bladder, prostate, urethra, penis, testis, gynecological organs, ovaries, breast, endocrine system, skin central nervous system; sarcomas of the soft tissue and bone; and melanoma of cutaneous and intraocular origin.

The term "hematological malignancies" includes childhood leukemia and lymphomas, Hodgkin's disease, lymphomas of lymphocytic and cutaneous origin, acute and chronic leukemia, plasma cell neoplasm and cancers associated with AIDS.

In addition, a cancer at any stage of progression can be treated, such as primary, metastatic, and recurrent cancers. In some embodiments, cancers are treated before metastasis is detected, for example, to inhibit metastatic cancer from developing. In other embodiments, cancers are treated when metastasis is detected, for example, to inhibit further metastasis and progression of the cancer.

The invention can also be used to treat autoimmune deficiency syndrome-associated Kaposi's sarcoma, cancer of the adrenal cortex, cancer of the cervix, cancer of the endometrium, cancer of the esophagus, cancer of the head and neck, cancer of the liver, cancer of the pancreas, cancer of the prostate, cancer of the thymus, carcinoid tumors, chronic lymphocytic leukemia, Ewing's sarcoma, gestational trophoblastic tumors, hepatoblastoma, multiple myeloma, non-small cell lung cancer, retinoblastoma, or tumors in the ovaries. A cancer at any stage of progression can be treated or detected, such as primary, metastatic, and recurrent cancers. Information regarding numerous types of cancer can be found, *e.g.*, from the American Cancer Society (www.cancer.org), or from, *e.g.*, Wilson et al. (1991) Harrison's Principles of Internal Medicine, 12th Edition, McGraw-Hill, Inc.

As used herein the terms "normal mammalian cell" and "normal animal cell" are defined as a cell that is growing under normal growth control mechanisms (*e.g.*, genetic control) and that displays normal cellular differentiation and normal migration patterns. Cancer cells differ from normal cells in their growth patterns, migration and in the nature of their cell surfaces. For example cancer cells tend to

grow continuously and chaotically, without regard for their neighbors, and can migrate to distal sites to generate tumors in other areas of the body (i.e., metastasize).

The present invention is directed, in some embodiments, to methods of treating or inhibiting metastatic cancer in an animal, for example, for human and veterinary uses, which include administering to a subject animal (e.g., a human), a therapeutically effective amount of an agent (e.g. a migrastatin analog, an inhibitory nucleic acid or an anti-fascin antibody) of the present invention.

Treatment of, or treating, a disease (e.g., cancer) is intended to include the alleviation of or diminishment of at least one symptom typically associated with the disease. The treatment also includes alleviation or diminishment of more than one symptom. The treatment may cure the disease, for example, by eliminating the symptoms and/or the source of the disease or condition. For example, treatment can cure the cancer by substantially inhibiting metastasis of the cancer cells so that removal or killing of the primary tumor or cancer cell(s) substantially eliminates the cancer. Treatment can also arrest or inhibit the metastasis of the cancer and/or tumor cells without directly killing or promoting the apoptosis of cancer cells.

Fascin functions in a variety of cellular functions that play critical roles in modulating the growth, movement and interaction of cells. However the actin bundling function of fascin is directly involved in tumor metastasis and invasive growth.

The anti-metastatic activity of fascin (e.g., in the presence of various test agents or therapeutic agents like those described herein) can be evaluated against varieties of cancers using methods described herein and available to one of skill in the art. Anti-cancer activity, for example, can be determined by identifying the dose that inhibits 50% cancer cell metastasis (GI50) of an agent of the invention.

The present invention also provides a method of evaluating a therapeutically effective dosage for treating a cancer (e.g., inhibiting metastasis) with an agent of the invention that includes determining the GI50 of the agent *in vitro*. Such a method permits calculation of the approximate amount of agent needed per volume

to inhibit cancer cell migration. Such amounts can be determined, for example, by standard microdilution methods.

In some embodiments, the agents of the invention can be administered in multiple doses over an extended period of time, or intermittently.

The term 'animal,' as used herein, refers to an animal, such as a warm-blooded animal, which is susceptible to or has a disease associated with fascin activity or expression, for example, metastatic cancer. Mammals include cattle, buffalo, sheep, goats, pigs, horses, dogs, cats, rats, rabbits, mice, and humans. Also included are other livestock, domesticated animals and captive animals. The term 'farm animals' includes chickens, turkeys, fish, and other farmed animals. Mammals and other animals including birds may be treated by the methods and compositions described and claimed herein.

Formulation and Administration

The compounds of the invention, including the compounds, migrastatin analogs, inhibitory nucleic acids, anti-fascin antibodies, test agents and candidate fascin modulators described herein, can be formulated as pharmaceutical compositions and administered to a mammalian host, such as a human patient in a variety of forms adapted to the chosen route of administration, i.e., orally or parenterally, by intravenous, intramuscular, topical or subcutaneous routes.

Inhibitory nucleic acids can be introduced into cells by a number of methods. In lipid-mediated transfection, cells take in non-covalent complexes between nucleic acid and a lipid or polymer reagent by endocytosis. Electroporation utilizes a brief electrical pulse to cause disruptions or holes in the cells' plasma membrane through which nucleic acid enters. Both of these methods successfully deliver any of the RNAi nucleic acids except viral vectors. Viral vector delivery occurs by infection of cells with the corresponding virus generated via a multi-step process. Viral vectors lack the ability to replicate themselves. Specialized cells express the missing genes necessary for viral replication and packaging. These cells produce and release virus into the culture medium upon conventional transfection with the viral vector. The virus containing the viral vector

is collected and purified. Infection of the desired cell line with virus introduces the siRNA or shRNA and knocks down gene expression. The viral delivery method absolutely requires the use of viral vectors and cannot accommodate the other sources of nucleic acid for RNAi.

Delivery of siRNA can be carried out by direct delivery of naked siRNA; encapsulation into liposomes and lipoplexes; conjugation to antibodies, peptides, aptamers, and other molecules; and formation of complexes with chemical and biological polymers. Intravenous, intraperetoneal, intranasal, and intratumoral siRNA administration can be carried out using polymer carriers and nanoparticles including PEI, low molecular weight PEI, chitosan, atelocollagen, transferrin targeted nanoparticles, liquid-targeted stabilized nanoparticles and dynamic polyconjugates.

Delivery of siRNA can further be carried out by conjugation of siRNA molecules to a targeting molecule including but not limited to proteins, peptides, and aptamers. In the case of peptides, a basic region, such as a poly-Arg stretch, is used (Kumar P, et al. Nature 2007 Jul 5;448(7149):39-43; Kim WJ, et al. Mol Ther 2006 Sep;14(3):343-350). For antibodies, conjugation to a protamine fusion protein can be used (Song E, et al. Nat Biotechnol 2005 Jun;23(6):709-717).

The present compounds including migrastatin analogs and inhibitory nucleic acids may be systemically administered, e.g., orally, in combination with a pharmaceutically acceptable vehicle such as an inert diluent or an assimilable edible carrier. They may be enclosed in hard or soft shell gelatin capsules, may be compressed into tablets, or may be incorporated directly with the food of the patient's diet. For oral therapeutic administration, the active compound may be combined with one or more excipients and used in the form of ingestible tablets, buccal tablets, troches, capsules, elixirs, suspensions, syrups, wafers, and the like. Such compositions and preparations should contain at least 0.1% of active compound. The percentage of the compositions and preparations may, of course, be varied and may conveniently be between about 2 to about 60% of the weight of a given unit dosage form. The amount of active compound in such therapeutically useful compositions is such that an effective dosage level will be obtained.

The tablets, troches, pills, capsules, and the like may also contain the following: binders such as gum tragacanth, acacia, corn starch or gelatin; excipients such as dicalcium phosphate; a disintegrating agent such as corn starch, potato starch, alginic acid and the like; a lubricant such as magnesium stearate; and a sweetening agent such as sucrose, fructose, lactose or aspartame or a flavoring agent such as peppermint, oil of wintergreen, or cherry flavoring may be added. When the unit dosage form is a capsule, it may contain, in addition to materials of the above type, a liquid carrier, such as a vegetable oil or a polyethylene glycol. Various other materials may be present as coatings or to otherwise modify the physical form of the solid unit dosage form. For instance, tablets, pills, or capsules may be coated with gelatin, wax, shellac or sugar and the like. A syrup or elixir may contain the active compound, sucrose or fructose as a sweetening agent, methyl and propylparabens as preservatives, a dye and flavoring such as cherry or orange flavor. Of course, any material used in preparing any unit dosage form should be pharmaceutically acceptable and substantially non-toxic in the amounts employed. In addition, the active compound may be incorporated into sustained-release preparations and devices.

The active compounds described herein may also be administered intravenously or intraperitoneally by infusion or injection. Solutions of the active compound or its salts can be prepared in water, optionally mixed with a nontoxic surfactant. Dispersions can also be prepared in glycerol, liquid polyethylene glycols, triacetin, and mixtures thereof and in oils. Under ordinary conditions of storage and use, these preparations contain a preservative to prevent the growth of microorganisms.

The pharmaceutical dosage forms suitable for injection or infusion can include sterile aqueous solutions or dispersions or sterile powders comprising the active ingredient which are adapted for the extemporaneous preparation of sterile injectable or infusible solutions or dispersions, optionally encapsulated in liposomes. In all cases, the ultimate dosage form should be sterile, fluid and stable under the conditions of manufacture and storage. The liquid carrier or vehicle can be a solvent or liquid dispersion medium comprising, for example, water, ethanol, a

polyol (for example, glycerol, propylene glycol, liquid polyethylene glycols, and the like), vegetable oils, nontoxic glyceryl esters, and suitable mixtures thereof. The proper fluidity can be maintained, for example, by the formation of liposomes, by the maintenance of the required particle size in the case of dispersions or by the use of surfactants. The prevention of the action of microorganisms can be brought about by various antibacterial and antifungal agents, for example, parabens, chlorobutanol, phenol, sorbic acid, thimerosal, and the like. In many cases, it will be preferable to include isotonic agents, for example, sugars, buffers or sodium chloride. Prolonged absorption of the injectable compositions can be brought about by the use in the compositions of agents delaying absorption, for example, aluminum monostearate and gelatin.

Sterile injectable solutions are prepared by incorporating the active compound in the required amount in the appropriate solvent with several of the other ingredients enumerated above, as required, followed by filter sterilization. In the case of sterile powders for the preparation of sterile injectable solutions, the preferred methods of preparation are vacuum drying and the freeze drying techniques, which yield a powder of the active ingredient plus any additional desired ingredient present in the previously sterile-filtered solutions.

For topical administration, the present compounds may be applied in pure form, i.e., when they are liquids. However, it will generally be desirable to administer them to the skin as compositions or formulations, in combination with a dermatologically acceptable carrier, which may be a solid or a liquid.

Useful solid carriers include finely divided solids such as talc, clay, microcrystalline cellulose, silica, alumina and the like. Useful liquid carriers include water, alcohols or glycols or water-alcohol/glycol blends, in which the present compounds can be dissolved or dispersed at effective levels, optionally with the aid of non-toxic surfactants. Adjuvants such as fragrances and additional antimicrobial agents can be added to optimize the properties for a given use. The resultant liquid compositions can be applied from absorbent pads, used to impregnate bandages and other dressings, or sprayed onto the affected area using pump-type or aerosol sprayers.

Thickeners such as synthetic polymers, fatty acids, fatty acid salts and esters, fatty alcohols, modified celluloses or modified mineral materials can also be employed with liquid carriers to form spreadable pastes, gels, ointments, soaps, and the like, for application directly to the skin of the user.

Examples of useful dermatological compositions which can be used to deliver the compounds of the invention to the skin are known to the art; for example, see Jacquet et al. (U.S. Pat. No. 4,608,392), Geria (U.S. Pat. No. 4,992,478), Smith et al. (U.S. Pat. No. 4,559,157) and Wortzman (U.S. Pat. No. 4,820,508).

Useful dosages of the compounds of the invention can be determined by comparing their *in vitro* activity, and *in vivo* activity in animal models. Methods for the extrapolation of effective dosages in mice, and other animals, to humans are known to the art; for example, see U.S. Pat. No. 4,938,949.

Generally, the concentration of the compound(s) of the invention in a liquid composition, such as a lotion, will be from about 0.01-25 wt-%, preferably from about 0.1-10 wt-%. The concentration in a semi-solid or solid composition such as a gel or a powder will be about 0.01-10 wt-%, preferably about 0.1-5 wt-%.

The amount of the compound, or an active salt or derivative thereof, required for use in treatment will vary not only with the particular salt selected but also with the route of administration, the nature of the condition being treated and the age and condition of the patient and will be ultimately at the discretion of the attendant physician or clinician. In general, however, a suitable dose will be in the range of from about 1.0 to about 200 mg/kg, e.g., from about 1 to about 100 mg/kg of body weight per day, such as about 2.0 to about 100 mg/kg of body weight per day, such as about 3.0 to about 50 mg per kilogram body weight of the recipient per day, preferably in the range of about 5 to 20 mg/kg/day. Alternatively, the compositions can be administered five times a week on five consecutive days with a two day rest, or four times a week on four consecutive days with a three day rest, or every other day.

Methods for extrapolating effective dosages in mice and other animals, to humans are known in the art (See, for example, U. S. Patent No. : 4,938,949). For example, in certain embodiments, compounds of the invention (for example those useful for the treatment of colon and/or ovarian cancer) may be administered at dosage levels of about

0.01 mg/kg to about 300 mg/kg, from about 0.1 mg/kg to about 250 mg/kg, from about 1 mg/kg to about 200 mg/kg, from about 1 mg/kg to about 150 mg/kg, from about 1 mg/kg to about 100 mg/kg, from about 1 mg/kg to about 90 mg/kg, from about 1 mg/kg to about 80 mg/kg, from about 1 mg/kg to about 70 mg/kg, from about 1 mg/kg to about 60 mg/kg, from about 1 mg/kg to about 50 mg/kg, from about 1 mg/kg to about 40 mg/kg, from about 1 mg/kg to about 30 mg/kg, from about 1 mg/kg to about 20 mg/kg, from about 5 mg/kg to about 100 mg/kg, from about 5 mg/kg to about 90 mg/kg, from about 5 mg/kg to about 80 mg/kg, from about 5 mg/kg to about 70 mg/kg, from about 5 mg/kg to about 60 mg/kg, from about 5 mg/kg to about 50 mg/kg, from about 5 mg/kg to about 40 mg/kg, from about 5 mg/kg to about 30 mg/kg, from about 5 mg/kg to about 20 mg/kg, from about 10 mg/kg to about 100 mg/kg, from about 10 mg/kg to about 90 mg/kg, from about 10 mg/kg to about 80 mg/kg, from about 10 mg/kg to about 70 mg/kg, from about 10 mg/kg to about 60 mg/kg, from about 10 mg/kg to about 50 mg/kg, from about 10 mg/kg to about 40 mg/kg, from about 10 mg/kg to about 30 mg/kg, from about 10 mg/kg to about 20 mg/kg, from about 20 mg/kg to about 100 mg/kg, from about 20 mg/kg to about 90 mg/kg, from about 20 mg/kg to about 80 mg/kg, from about 20 mg/kg to about 70 mg/kg, from about 20 mg/kg to about 60 mg/kg, from about 20 mg/kg to about 50 mg/kg, from about 20 mg/kg to about 40 mg/kg, from about 20 mg/kg to about 30 mg/kg, of subject body weight per day, one or more times a day, to obtain the desired therapeutic effect. In certain embodiments, compounds may be administered at a dosage of about 1 mg/kg or greater, 5 mg/kg or greater; 10 mg/kg or greater, 15 mg/kg or greater, 20 mg/kg or greater, 25 mg/kg or greater, 30 mg/kg or greater, 35 mg/kg or greater, 40 mg/kg or greater, 45 mg/kg or greater, 50 mg/kg or greater, 60 mg/kg or greater, 70 mg/kg or greater, of body weight. It will also be appreciated that dosages smaller than 0.01 mg/kg or greater than 70 mg/kg (for example 70-200 mg/kg) can be administered to a subject.

In certain embodiments, compounds may be used in chemotherapy (i.e., to inhibit metastasis) and may be administered at higher dosage. For example, compounds to be used in chemotherapy may be administered from about 100 mg/kg to about 300 mg/kg, from about 120 mg/kg to about 280 mg/kg, from about 140 mg/kg to about 260 mg/kg, from about 150 mg/kg to about 250 mg/kg, from about 160 mg/kg to about 240 mg/kg, of

subject body weight per day, one or more times a day, to obtain the desired therapeutic effect.

In certain other embodiments, compounds may be used in supportive therapy (e. g., as an adjuvant to surgery or irradiation in a range of common types of tumor) and may be administered at lower dosage. For example, compounds to be used in supportive therapy may be administered from about 1 mg/kg to about 30 mg/kg, from about 1 mg/kg to about 25 mg/kg, from about 5 mg/kg to about 20 mg/kg, of subject body weight per day, one or more times a day, to obtain the desired therapeutic effect.

In certain other embodiments, compounds may be used for preventing and/or treating metastatic cancer (e. g., ovarian and/or colon cancer) and may be administered at an intermediate dosage. For example, compounds to be used in supportive therapy may be administered from about 1 mg/kg to about 100 mg/kg, from about 1 mg/kg to about 80 mg/kg, from about 5 mg/kg to about 70 mg/kg, from about 10 mg/kg to about 70 mg/kg, from about 10 mg/kg to about 60 mg/kg, from about 20 mg/kg to about 70 mg/kg, from about 20 mg/kg to about 60 mg/kg, of subject body weight per day, one or more times a day, to obtain the desired therapeutic effect.

The compound is conveniently administered in unit dosage form; for example, containing 45 to 3000 mg, conveniently 90 to 2250 mg, most conveniently, 450 to 1500 mg of active ingredient per unit dosage form. In some embodiments, the compound is administered at dosages of about 1 to about 100 mg/kg.

Ideally, the active ingredient should be administered to achieve peak plasma concentrations of the active compound of from about 0.5 nM to about 10 μM, preferably, about 1 nM to 1 μM, most preferably, about 10 nM to about 0.5 μM. This may be achieved, for example, by the intravenous injection of a 0.05 to 5% solution of the active ingredient, optionally in saline, or orally administered as a bolus containing about 20-2000 mg of the active ingredient. Desirable blood levels may be maintained by continuous infusion to provide about 0.2 to 1.0 mg/kg/hr or by intermittent infusions containing about 0.4 to 20 mg/kg of the active ingredient(s).

The desired dose may conveniently be presented in a single dose or as divided doses administered at appropriate intervals, for example, as two, three, four or more sub-doses per day. The sub-dose itself may be further divided, e.g., into a number of discrete

loosely spaced administrations; such as multiple inhalations from an insufflator or by application of a plurality of drops into the eye.

Compounds of the invention are useful as therapeutic agents administered for inhibition of cell migration and treatment of metastatic cancer. Such cancers include but are not limited to, cancers involving the animal's head, neck, lung, mesothelioma, mediastinum, esophagus, stomach, pancreas, hepatobiliary system, small intestine, colon, colorectal, rectum, anus, kidney, ureter, bladder, prostate, urethra, penis, testis, gynecological organs, ovaries, breast, endocrine system, skin, or central nervous system. Thus, for example, the cancer can be a breast cancer, a leukemia, a lung cancer, a colon cancer, a central nervous system cancer, a melanoma, an ovarian cancer, a renal cancer, or a prostate cancer.

Additionally, compounds of the invention may be useful as pharmacological tools for the further investigation of the inhibition of cell migration.

The compounds of the invention can also be administered in combination with other therapeutic agents that are effective for treating or controlling the spread of cancerous cells or tumor cells.

Moreover, the compounds of the invention can be tested in appropriate animal models. For example, the compounds of the invention can be tested in animals with known tumors, or animals that have been injected with tumor cells into a localized area. The degree or number of secondary tumors that form over time is a measure of metastasis and the ability of the compounds to inhibit such metastasis can be evaluated relative to control animals that have the primary tumor but receive no test compounds. Experimental results from this type of *in vivo* testing are shown in FIG. 8 and are further described in the Examples. These results demonstrate that the compounds of the invention substantially reduce or eliminate tumor metastasis.

The compounds of the invention will also find use in treatment of brain disorders (Kraft et al., Phenotypes of Drosophila brain neurons in primary culture reveal a role for fascin in neurite shape and trajectory. J. Neurosci. (2006)); Hodgkin's disease (Pinkus et al., Fascin, a sensitive new marker for Reed-Sternberg cells of Hodgkin's disease. Evidence for a dendritic or B cell derivation? Am. J. Pathol. (1997)); virus infection (Mosialos et al., Circulating human dendritic cells differentially express high levels of a

55-kd actin-bundling protein. Am. J. Pathol. (1996)); neuronal degeneration (Fulga et al., Abnormal bundling and accumulation of F-actin mediates tau-induced neuronal degeneration in vivo. Nat Cell Biol. 2007 Feb;9(2):139-48)); lymphoid hyperplasia (Said et al., The role of follicular and interdigitating dendritic cells in HIV-related lymphoid hyperplasia: localization of fascin. Mod Pathol. 1997 May;10(5):421-7)); and ischemia (Meller et al., Ubiquitin proteasome-mediated synaptic reorganization: a novel mechanism underlying rapid ischemic tolerance. J Neurosci. 2008 Jan 2;28(1):50-9.))

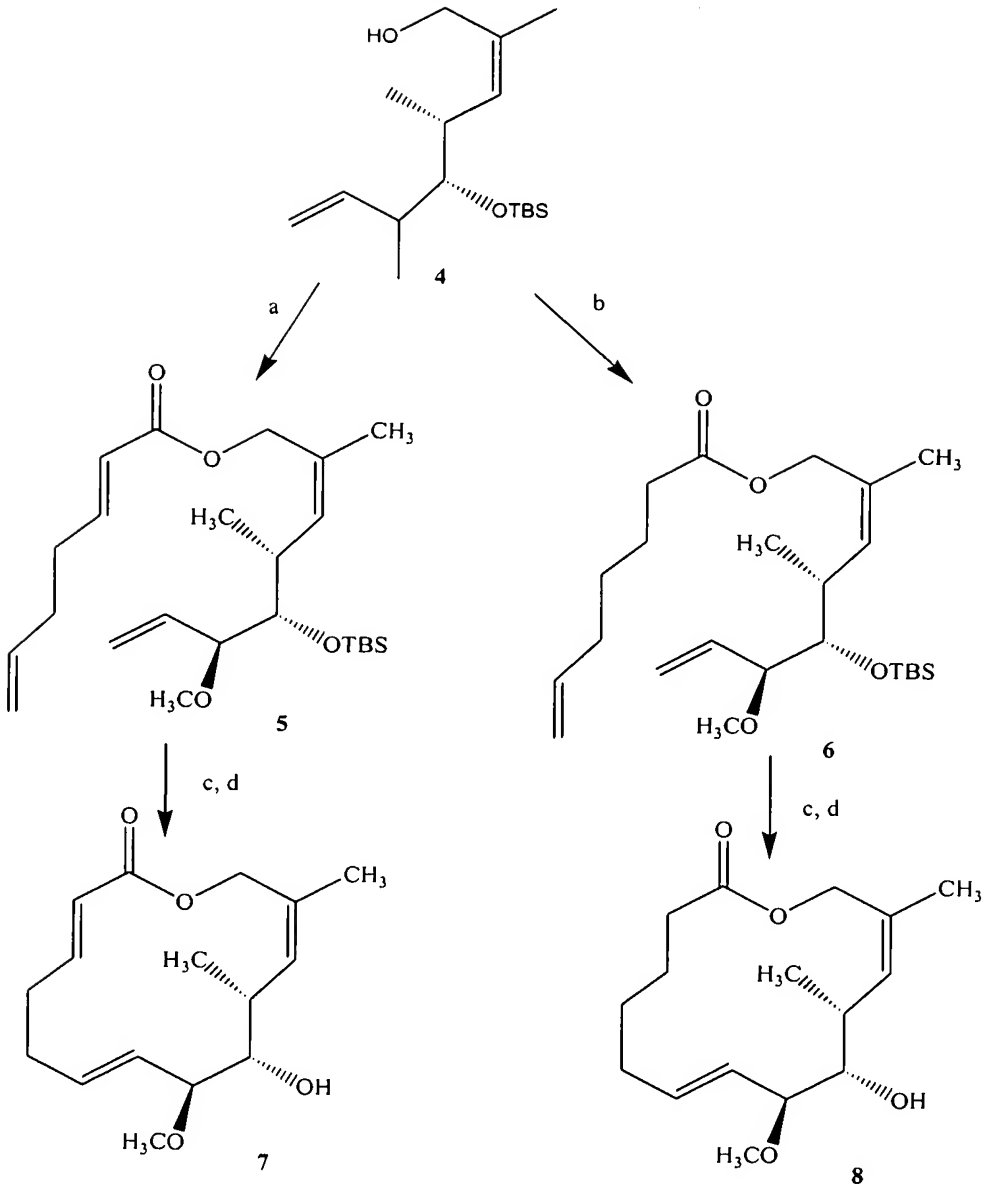
The invention will now be illustrated by the following non-limiting Examples.

Example 1

Chemical Synthesis and Characterization

This Example describes the synthesis as well as the chemical and physical characterization of compounds.

Synthesis: Compounds of the invention can be synthesized as shown below.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5
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c, d
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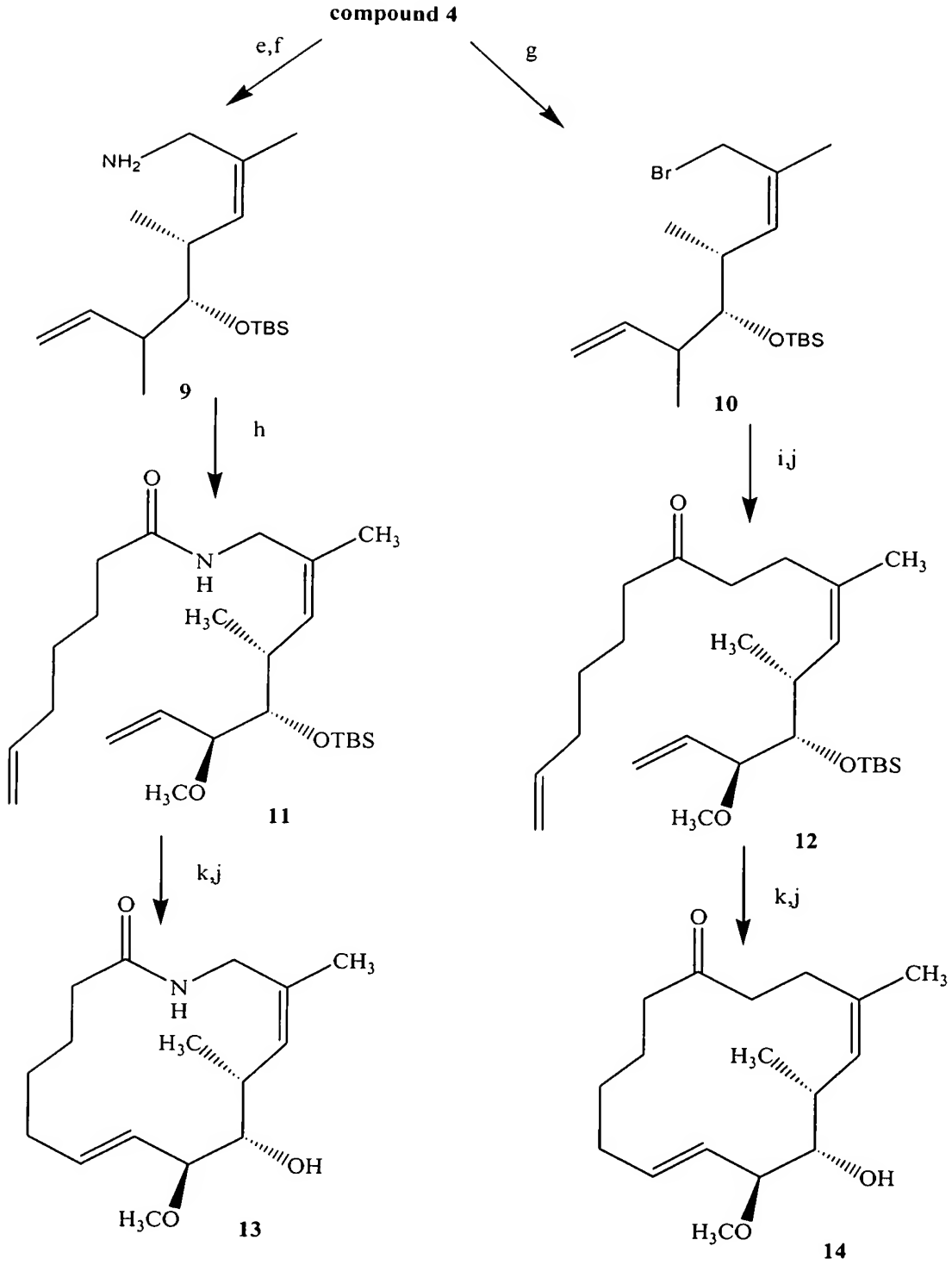
compound 4
e,f
g
NH2
OTBS
9
Br
OTBS
10
h
i,j
O
N
H
CH3
H3C
OTBS
H3CO
11
12
k,j
k,j
OH
13
14

The reagents and conditions employed are as follows: (a) Yamaguchi acylation (48%); (b) Et_3N, DMAP, 6-heptenoyl chloride (89%); (c) Grubbs catalyst, toluene and reflux (47 and 73%); (d) HF-pyridine, THF (78 and 90%); (e) diphenylphosphoryl azide (87%); (f) PPh_3, H_2O (90%); (g) CBr_4, PPh_3 (95%); (h) EDCI, 6-heptenioc acid (70%); (i) 1-benzenesulfonyl-oct-7-en-one, DBU (75%); (j) Na/Hg (79%); (k) Grubbs catalyst, toluene, reflux (70 and 75%); (l) HF-pyridine, THF (90 and 95%).

Analytical Equipment: Optical rotations are measured on a JASCO DIP-370 digital polarimeter at room temperature. Concentration (*c*) in g/100 ml and solvent are given in parentheses. Infrared spectra are obtained on a Perkin-Elmer 1600 FT-IR spectrophotometer neat or as a film in $CHCl_3$ (NaCl plates). Absorption bands are noted in cm_{-1}. ^1H- and ^{13}C-NMR spectra are recorded on a Bruker AMX-400 MHz or a Bruker Advance DRX-500 MHz spectrometer in CDCl3 (referenced to 7.26 ppm (δ) for ^1H-NMR and 77.0 ppm for ^{13}C-NMR). Coupling constants (*J*) (H,H) are given in Hz, spectral splitting patterns are designated as singlet (s), doublet (d), triplet (t), quadruplet (q), multiplet or more overlapping signals (m), apparent (app), broad signal (br). Low resolution mass spectra (ionspray, a variation of electrospray) are acquired on a Perkin-Elmer Sciex API 100 spectrometer. Samples are introduced by direct infusion. High resolution mass spectra (fast atom bombardment, FAB) are acquired on a Micromass 70-SE-4F spectrometer.

Migrastatin core 7: $[\alpha]_D$ +106.0° (*c* 0.50, CHCl3); IR ($CHCl_3$) 3567, 2933, 2881, 1716, 1602, 1448, 1393, 1255, 1107, 1052; ^1H-NMR (500 MHz, CDCl3) δ 6.81-6.75 (m, 1H), 5.73 (d, J = 15.9, 1H), 5.62-5.55 (m, 2H), 5.14 (dd, J = 15.2, 6.8, 1H), 4.72 (d, J = 15.6, 1H), 4.63 (d, J = 15.6, 1H), 3.42-3.38 (m, 2H), 3.28 (s, 3H), 3.03-2.97 (m, 1H), 2.69 (br s, 1H), 2.47-2.38 (m, 2H), 2.32-2.18 (m, 2H), 1.68 (s, 3H), 0.88 (d, J = 6.9, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 165.36, 149.52, 133.85, 129.79, 129.51, 127.50, 122.15, 84.62, 76.09, 65.40, 56.25, 32.20, 31.34, 29.99, 22.27, 12.66; MS (ESI) 303 [M+Na^+]; HRMS (FAB) calcd. for $C_{16}H_{24}O_4$ [M+Na^+] 303.1571, found 303.1572.

2,3-Dihydro-migrastatin core 8: $[\alpha]_D$ +115.3° (*c* 1.00, $CHCl_3$); IR ($CHCl_3$) 3567, 3016, 2933, 2858, 1724, 1450, 1387, 1317, 1258, 1145, 1115, 979; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 5.74-5.67 (m, 2H), 5.23 (dd, *J* = 15.7, 7.7, 1H), 4.54 (d, *J* = 13.1, 1H), 4.29 (d, *J* = 13.1, 1H), 3.46-3.39 (m, 2H), 3.30 (s, 3H), 2.82-2.77 (m, 1H), 2.44-2.39 (m, 1H), 2.26-2.15 (m, 2H), 2.03-1.97 (m, 1H), 1.74 (d, *J* = 0.9, 3H), 1.74-1.70 (m, 1H), 1.60-1.52 (m, 2H), 1.36-1.32 (m, 1H), 0.93 (d, *J* = 6.9, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 173.69, 135.19, 134.39, 129.02, 127.14, 83.82, 75.91, 64.76, 56.34, 34.23, 32.06, 29.88, 27.20, 23.40, 23.27, 12.81; MS (ESI) 305 [M+Na^+]; HRMS (FAB) calcd. for $C_{16}H_{26}O_4$ [M+Na^+] 305.1719, found 305.1729.

Migrastatin lactam 13: $[\alpha]_D$ +101.3° (*c* 1.00, $CHCl_3$); IR ($CHCl_3$) 3566, 3444, 3021, 2936, 2828, 1658, 1504, 1478, 1398, 1229, 1088, 979; ^{1}H-NMR (500 MHz, $CDCl_3$) ä 5.79-5.73 (m, 1H), 5.66 (d, *J* = 10.2, 1H), 5.24 (dd, *J* = 15.8, 7.5, 1H), 5.12 (br s, 1H), 3.91 (dd, *J* = 13.7, 4.1, 1H), 3.50-3.46 (m, 2H), 3.34-3.30 (m, 1H), 3.31 (s, 3H), 2.89 (br s, 1H), 2.56-2.52 (m, 1H), 2.32-2.25 (m, 2H), 2.16-2.11 (m, 1H), 1.96-1.89 (m, 1H), 1.77 (d, *J* = 1.1, 3H), 1.73-1.51 (m, 3H), 1.37-1.32 (m, 1H), 0.94 (d, *J* = 6.9, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 173.36, 135.52, 133.77, 129.89, 128.73, 83.21, 76.38, 56.45, 41.40, 35.95, 32.27, 29.86, 27.00, 24.82, 24.42, 13.03; MS (ESI) 304 [M+Na^+]; HRMS (FAB) calcd. for C16H27NO3 [M+Na^+] 304.1888, found 304.1889.

Migrastatin ketone (14): $[\alpha]_D$ +77.0° (*c* 0.5, $CHCl_3$); IR (neat) 3566, 3022, 3015, 2975, 2937, 2879, 1700, 1448, 1384, 1237, 1109, 1085, 979 cm-1; ^{1}H-NMR (500 MHz, $CDCl_3$) ä 5.72 (ddd, *J* = 15.0, 8.5, 6.0, 1H), 5.37 (dd, *J* = 10.0, 0.9 1H), 5.31 (dd, *J* = 15.6, 7.8, 1H), 3.47 (t, *J* = 8.5, 1H), 3.36 (dd, *J* = 9.2, 1.2, 1H), 3.31 (s, 3H), 2.78 (br s, 1H), 2,51-2,45 (m, 2H), 2,37-2.32 (m, 2H), 2,26-2,16 (m, 5H), 1.69 (d, *J* = 1.3, 3H), 1.69-1.59 (m, 2H), 1.53-1.50 (m, 2H), 0.95 (d, *J* = 6.8, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 212.10, 135.23, 132.91, 130.26, 129.22, 83.69, 77.62, 56.45, 42.08, 40.67, 32.57, 30.33, 28.57, 27.01, 23.22, 23.14, 12.61; MS (ESI) 303 [M+Na^+]; HRMS (FAB) calcd. for C17H28O3Na [M+Na^+] 303.1936, found 303.1938.

(R)-Isopropyl migrastatin (17): $[\alpha]_D$ +21.3° (*c* 0.09, CHCl3); IR (neat) 3499, 2967, 2926, 2866, 1729, 1453, 1383, 1257, 1111, 981 cm-1; ^{1}H-NMR (500 MHz, $CDCl_3$) ä 5.65 (dt, *J* = 15.5, 7.5, 1H), 5.58 (dd, *J* = 10.7, 1.3, 1H), 5.35 (dd, *J* = 15.5, 6.0, 1H), 4.87 (d, *J* = 7.6, 1H), 3.49 (dd, *J* = 9.1, 6.0, 1H), 3.34 (s, 3H), 3.27 (br d, *J* = 8.8, 1H), 3.13-3.07 (m, 1H), 2.86, (br s, 1H), 2.34-2.15 (m, 4H), 2.06-1.99 (m, 1H), 1.76 (d, *J* = 1.6, 3H), 1.75-1.58 (m, 3H), 1.47-1.41 (m, 1H), 0.98 (d, *J* = 7.0, 3H), 0.93 (d, *J* = 6.7, 3H), 0.92 (d, *J* = 6.7, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 172.50, 132.45, 132.08, 131.58, 128.26, 82.45, 80.74, 77.44, 33.00, 32.66, 31.76, 30.56, 25.57, 24.91, 22.44, 19.02, 18.96, 13.20; MS (ESI) 324 [M+Na^+]; HRMS (FAB) calcd. for $C_{19}H_{32}O_4Na$ [M+Na^+] 347.2198, found 347.2196.

(S)-Isopropyl migrastatin (18): $[\alpha]_D$ +25.1° (*c* 0.32, $CHCl_3$); IR (neat) 3479, 2967, 2926, 2876, 1724, 1448, 1373, 1257, 1237, 1091, 976 cm-1; ^{1}H-NMR (500 MHz, $CDCl_3$) ä 5.70 (ddd, *J* = 15.4, 8.5, 5.3, 1H), 5.33 (dd, *J* = 10.0, 0.9, 1H), 5.30 (d, *J* = 7.0, 1H) 5.19-5.13 (m, 1H), 3.40-3.30 (m, 2H), 3.28 (s, 3H), 2.99-2.96 (m, 1H), 2.76 (s, 1H), 2.36-2.24 (m, 2H), 2.20-2.08 (m, 2H), 1.99 (dt, *J* = 7.0, 6.9, 1H) 1.69 (d, *J* = 1.3, 3H), 1.62-1.52 (m, 4H), 0.94 (d, *J* = 7.0, 3H), 0.91 (d, *J* = 6.6, 3H), 0.86 (d, *J* = 6.9, 3H); ^{13}C-NMR (125 MHz, CDCl3) δ 172.97, 135.94, 133.83, 130.09, 127.75, 86.47, 78.70, 55.98, 33.99, 32.80, 30.38, 29.82, 27.34, 22.57, 21.38, 19.09, 18.05, 15.20; MS (ESI) 324 [M+Na^+]; HRMS (FAB) calcd. for C19H32O4Na [M+Na^+] 347.2198, found 347.2187.

Example 2

Inhibition of Metastatic Tumor Cell Migration by Migrastatin Analogs

The efficacy of the compounds of the invention for inhibiting cell migration was assessed using two procedures, a wound healing assay and a chamber cell migration assay.

Methods

Cells. Mouse 4T1 mammary tumor cells and human MDA-MB-231 breast tumor cells were obtained from ATCC and have been described previously (Shan et al. 2005, Yang et

al. 2005). 4T1 cells were cultured in RPMI 1640 medium supplemented with 10% FBS. MDA-MB-231 cells were cultured in DMEM supplemented with 10% FBS.

Wound-healing assay. The wound-healing assay involves observing whether confluent cells can migrate across a scrape or wound in the cell layer. Cell migration assays were performed as described previously (Yang et al. 2005, Shan et al 2006). Tumor cells were plated in a 24-well plate coated with gelatin in standard media. After the cells grew to confluence, wounds were made in the confluent layer of cell using a sterile instrument such as a sterile pipette tip. The cells were washed with Phosphate Buffered Saline (PBS) or other sterile solutions and then the migration was induced by adding medium supplemented with 10% FBS. When the wound for the positive control closed, cells were fixed with 3.7% formaldehyde and stained with crystal violet staining solution. Compounds that inhibit the migration of cells into the wound area at low concentrations are useful for inhibiting cell migration and treating metastatic cancer.

Chamber cell migration assay. The chamber cell migration assay assesses whether cell can migrate through a filter having pores of known sizes. For example, cell migrations can be assayed with Boyden chambers having filters with about 8.0 μm pore size. Briefly, cells in serum-free medium are added to the first chamber and 500 μl of medium with 10% fetal bovine serum (FBS) is added to the second chamber. The chamber is incubated for about 6-8 hours at 37°C with different concentrations of chemical compounds in both of the two chambers. Cells in the first chamber are removed with a cotton swab, and cells in the other chamber or on the other side of the filter are fixed and stained. Photographs several random regions of the filter facing the second chamber are taken and the number of cells counted to calculate the average number of cells that had transmigrated.

Results

The effects of the core macroketone and the core macrolactam analogs on the migration of tumor cells in vitro were studied. As shown in FIG. 1, while serum induced the migration of metastatic mouse breast tumor 4T1 cells, the addition of the macroketone or macrolactam congeners inhibited serum-induced 4T1 cell migration as measured by both the wound-healing assay and the Boyden chamber assay (FIG. 1B-D). The macroketone and macrolactam core structures were quite effective with IC_{50} values

of 100 and 255 nM, respectively (FIG. 1C and 1D). The parent compound migrastatin had an IC50 of 29 μM (Njardarson et al. 2004, Gaul et al. 2004). These compounds had little effect on the proliferation of 4T1 cells in culture (*Id.*).

The macroketone and macrolactam congeners also inhibited the migration of several invasive and metastatic human tumor cell lines, such as human breast tumor MDA-MB 231 cells, human prostate tumor PC-3 cells, and human colon tumor Lovo cells (FIG. 2A and B). In contrast, migration of normal human mammary gland epithelia MCF-10A cells, mouse embryonic fibroblast cells, or primary mouse leukocytes was rather insensitive to these compounds (FIG. 2C and D). These cellular studies demonstrated that the macroketone and macrolactam core structures are highly selective for mouse and human metastatic tumor cells versus normal cells. These results also suggest that the level or activity of the biochemical target of these compounds might be high in metastatic tumor cells thus sensitizing these tumor cells to the compounds.

Example 3

Inhibition of Lung Metastasis of Highly Metastatic Mammary Carcinoma Cells by Migrastatin Analogs in Mice

The analogs were tested to determine if they could affect tumor metastasis in the 4T1 mouse mammary tumor model. The lung metastasis of 4T1 tumor cells in mice with or without treatment with these chemical compounds was examined. The mouse 4T1 tumor closely mimics human breast cancer in its anatomical site, immunogenicity, growth characteristics, and metastatic properties (Pulaski et al. 1998). From the mammary gland, the 4T1 tumor spontaneously metastasizes to a variety of target organs including the lung, bone, brain, and liver (Aslakson et al. 1992). Ten days after implantation of 4T1 cells (1×10^5) in the mammary glands of BALB/c mice, the mice were injected intraperitoneally with the macroketone and the macrolactam core structures, or control saline PBS. The dosages of the macroketone or macrolactam core structures were 10 mg/kg or 20 mg/kg. The compounds were injected. After 20 days, the mice were sacrificed and metastasis to the lung was examined by clonogenic assay (Shen et al., 2005). While mice injected with the control saline (vehicle alone) showed large numbers of metastasized 4T1 cells in the lung, the number of metastasized 4T1 cells in

the lungs of mice treated with either macroketone or macrolactam was reduced by 91%–99% (FIG. 3A). Mice treated with macroketone or macrolactam formed primary mammary tumors similar in size to those of mice treated with saline (FIG. 3C), implying that these chemical compounds did not interfere with primary tumor formation by 4T1 cells. These compounds did not cause obvious side effects since the mice appeared normal with no evidence of weight loss, lethargy, or ruffled fur. These results demonstrate that the macroketone and macrolactam are potent inhibitors of 4T1 tumor cell metastasis from the mammary gland to the lung.

As further controls for the specific effects of these core structures, two other compounds were examined: migrastatin semi-core and macrolactone (FIG. 3B). Upon testing with 4T1 cells for its ability to inhibit cell migration in vitro, migrastatin semi-core showed a significantly lower activity than macroketone and macrolactam with an IC_{50} of 40 μM (Njardarson et al. 2004, Gaul et al. 2004). Although the macrolactone was very effective at inhibiting 4T1 cell migration (IC_{50} of 24 nM), previous metabolic stability studies showed that it was very unstable in mouse plasma with a half-life of < 5 minutes (Gaul et al. 2004). As shown in FIG. 3A, treatment of mice with migrastatin semi-core (10 and 20 mg/kg) did not significantly reduce the 4T1 tumor metastasis in these mice. Although the effect of 20 mg/kg macrolactone on 4T1 tumor metastasis was statistically significant, it was much less than those of macroketone and macrolactam (FIG. 3A). The reduced effectiveness of macrolactone was likely due to its instability in mice.

Example 4

Inhibition of Lamellipodium Formation by Migrastatin Analogs

The effects of macroketone and macrolactam on the actin cytoskeleton and microtubules in 4T1 cells was examined. Cell migration is a sequential and interrelated multi-step process (Ridley et al. 2003). It involves the formation of lamellipodia at the front edge, cycles of adhesion and detachment, cell body contraction, and tail retraction (Ridley et al. 2003). The core macroketone and the core macrolactam inhibited the formation of lamellipodia at the leading edge (Shan et al. 2005). While the addition of serum induced the formation of lamellipodia, addition of either the macroketone or

macrolactam cores disrupted the formation of lamellipodia (Shan et al. 2005). Moreover, neither compound had any effect on the microtubule organization. These data demonstrated that the cellular basis of the action of these migrastatin analogs on tumor metastasis involves the disruption of actin cytoskeletal reorganization.

Example 5

Migrastatin Analogs Inhibit the Actin-Bundling Activity of Fascin

Methods

Identification of fascin as the protein target of migrastatin analogs. Whole cell lysates from 4T1 mouse breast tumor cells were made. After preclearing the cell lysate with immobilized neutravidin biotin binding protein (Pierce, IL, USA) to remove biotin and avidin-binding proteins, the cell lysates were loaded to a column packed with the biotin-labeled macroketone (conjugated to neutravidin beads). A control column packed with free biotin and neutravidin beads was run side-by-side. After washing the column with 10 bed volumes of lysis buffer with 300 mM NaCl, the bound proteins were eluted with 0.1 M Glycine-HCl at pH 2.8 according to the manufacturer's instruction. From the SDS-PAGE, one band (~55 kDa) was specifically present in the sample eluted from the biotin-labeled macroketone column but not in the sample eluted from the biotin column. The band containing this ~55 kDa protein was cut out of the gel and the protein was identified as mouse fascin 1 by mass spectrometry.

Protein Expression and Purification. Recombinant GST-fascin fusion protein was produced in BL21 Escherichia coli. A 1-liter culture was grown to an A600 reading of 1.0 and then induced by addition of 0.3 mM isopropyl 1-thio-D-galactopyranoside (IPTG) for 12 hours at 25°C. Cells were flash frozen and then lysed by sonication in Tris-buffered saline. The supernatant was then incubated with glutathione-Sepharose for 2 h at 4°C. After extensive washing, GST-fascin was eluted and concentrated with a Centricon Plus-20 (Millipore). To remove the GST tag from the fusion protein, beads were incubated with thrombin overnight at 4°C. The supernatant was collected and concentrated.

GST-fascin and Biotin-macroketone Interaction. Purified recombinant fascin protein or control protein were incubated with biotin-macroketone for 2 h at 4°C. Proteins

associated with biotin-macroketone were precipitated with Untralink-immobilized NeutrAvidin agarose (Pierce). After extensive washing, bound proteins were eluted with SDS sample buffer and resolved by 10% SDS-PAGE.

F-Actin Bundling Assay. Actin bundling activity was measured by low speed centrifugation assay and fluorescence microscopy. In low-speed centrifugation assay, monomeric rabbit G-actin was induced to polymerize at room temperature in F-actin buffer (20 mM Tris–HCl at pH 8, 1 mM ATP, 1 mM DTT, 2 mM MgCl2 and 100 mM KCl). Recombinant fascin proteins or control buffer were subsequently incubated with F-actin for 60 min at room temperature and centrifuged for 30 min at 10,000g in an Eppendorf 5415D table-top centrifuge. Both supernatants and pellets were dissolved in an equivalent volume of SDS sample buffer, and the amount of actin was determined by SDS-PAGE. For fluorescence microscopy, monomeric G-actin was polymerized as described above. F-actin was mixed with recombinant fascin protein in F-buffer and incubated at room temperature for 30 min. Actin was then labeled by adding 5 % rhodamine–phalloidine to the mixture. The samples were mounted between a slide and a coverslip coated with poly-lysine and imaged by fluorescence microscopy.

F-Actin Binding Assay. Actin polymerization was performed as described above. Recombinant fascin proteins or control buffer were subsequently incubated with F-actin for 60 min at room temperature. Mixtures were centrifuged at 100,000 g (Beckman Airfuge) for 30 min. Both supernatants and pellets were dissolved in an equivalent volume of SDS sample buffer and analyzed by SDS-PAGE.

Immunofluorescence Microscopy. Cells cultured on gelatin-coated glass coverslips were fixed with 3.7% formaldehyde in PBS for 10 min at room temperature, permeabilized with 0.1% Triton X-100 for 5 min, and then washed with PBS three times. To block nonspecific binding, the cells were incubated with a solution of PBS containing 1% bovine serum albumin for 30 min and then incubated with primary antibody at appropriate dilutions for 1 h. After incubation with primary antibody, cells were washed three times with PBS and incubated with fluorescence-conjugated secondary antibody (Molecular Probes). The coverslips were then fixed onto slides and imaged using a Zeiss fluorescence microscope.

Electron Microscopy. Samples were absorbed onto freshly glow-discharged, carbon-coated copper grids for 2 minutes and stained with 2% uranyl acetate. Grids were examined using a Zeiss electron microscopy at an accelerating voltage of 80 kV.

Results

To understand the molecular basis of the action of migrastatin analogs, the protein target of migrastatin analogs was identified. An unbiased approach towards the identification of the protein target employing a biotin-labeled macroketone was tested (see FIG. 4A). This biotin-labeled migrastatin analog was active in inhibiting the 4T1 breast tumor cell migration (Gaul et al. 2004). The biotin-labeled macroketone was used to set up an affinity column and the ~55 kDa protein target was successfully purified (FIG. 4B) and identified as mouse fascin 1 by mass spectrometry.

Different but complementary approaches were used to verify fascin as the target. The first approach was in vitro studies on the interaction of migrastatin analogs with fascin. Fascin was purified as a GST-fusion protein from *Escherichia coli* (FIG. 5A and 5B). Purified fascin, but not GST control, specifically interacted with biotin-conjugated macroketone (FIG. 5A and 5B). Additionally, excess amount of non-biotinylated macroketone efficiently competed the binding between fascin and biotin-conjugated macroketone (FIG. 5C). Another migrastatin analog, macrolactam, also competed the binding of biotin-conjugated macroketone to fascin (data not shown). Collectively, these data demonstrate that fascin is a protein target of macroketone.

Three different approaches were used to investigate the effect of macroketone on fascin. First, the actin-bundling activity of purified recombinant fascin protein was investigated by the F-actin pelleting assay (Yamashiro-Matsumura et al. 1985). In this low-speed centrifugation assay, the pellets contain bundles of F-actin polymers. Purified fascin increased the amounts of F-actin bundles in the pellets (FIG. 6A). While macroketone alone had no effect on the formation of F-actin bundles, macroketone significantly decreased the fascin-induced bundling of F-actin polymers (FIG. 6A). Second, fluorescence microscopy was used to visualize the fascin-regulated F-actin filament bundles in the absence and presence of macroketone (FIG. 6B). Addition of fascin induced the formation of F-actin bundles, as revealed by the staining of F-actin filaments with Rhodamine-conjugated phalloidine (FIG. 6B). In contrast, in the presence

of macroketone, formation of F-actin bundles was largely (>80%) inhibited (FIG. 6B and 6C). Third, electron microscopy was used to examine the actin bundles (FIG. 6D). The EM examination revealed that macroketone decreased the thickness of the bundles (FIG. 6D). These thin F-actin bundles often had branches which were not observed in the absence of macroketone. For fascin to bundle F-actin polymers, fascin needs to bind to F-actin polymers. Thus, it is likely that macroketone inhibits the direct binding of fascin to F-actin. To confirm this, high-speed centrifugation method was used to pellet F-actin polymers (Yamashiro-Matsumura et al. 1985). Under these conditions, fascin alone was not precipitated and fascin could only be pulled-down by binding to F-actin polymers (Id.). While similar amounts of F-actin polymers were in the pellets in the absence and presence of macroketone (since the same amounts of F-actin polymers were added), significantly less fascin was pulled down by F-actin in the presence of macroketone (FIG. 6E). These data demonstrate that macroketone inhibits the actin-bundling activity of fascin.

Example 6

Essential Role for Fascin in Breast Tumor Cell Migration

Methods

RNA interference. RNAi of fascin was performed in 4T1 mouse breast tumor and MDA-MB-231 human breast tumor cells using pSUPER vector (Oligoengine). The target sequences of the two pairs of mouse fascin were GGTGGGCAAAGATGAGCTC (SEQ ID NO:63) and GTGGAGCGTGCACATCGCC (SEQ ID NO:64). The target sequences of the two pairs of human fascin were GGTGGGCAAGGACGAGCTC (SEQ ID NO:65) and GCCTGAAGAAGAAGCAGAT (SEQ ID NO:66). One day before transfection, cells were plated in 0.5 ml of growth medium without antibiotics. At the time of transfection, the cells were 30-50% confluent. For each transfection sample, siRNA was prepared as follows:

1) Dilute the appropriate amount of siRNA in 50 μl of Opti-MEM I Reduced Serum Medium without serum (or other medium without serum). Mix gently.

2) Mix Lipofectamine 2000 gently before use, then dilute the appropriate amount in 50 μl of Opti-MEMI Medium (or other medium without serum). Mix gently

and incubate for 5 minutes at room temperature. Note: Combine the diluted Lipofectamine 2000 with the diluted siRNA within 30 minutes. Longer incubation times may decrease activity. If D-MEM is used as a diluent for the Lipofectamine 2000, mix with the diluted siRNA within 5 minutes.

3) After the 5 minute incubation, combine the diluted siRNA with the diluted Lipofectamine 2000 (total volume is 100 μl). Mix gently and incubate for 20 minutes at room temperature to allow the siRNA:Lipofectamine 2000 complexes to form.

Add the 100 μl of siRNA:Lipofectamine 2000 complexes to each well. Mix gently by rocking the plate back and forth.

Cells were incubated at 37°C in a CO_2 incubator for 24-72 hours until they were ready to assay for gene knockdown. It was generally not necessary to remove the complexes or change the medium; however, growth medium was replaced after 4-6 hours without loss of transfection activity.

The following additional cell lines were likewise tested with migrastatin analogs and fascin siRNA as described herein: human colon tumor Lovo-229 cells; human prostate tumor PC-3 cells; melanoma B16 cells; ovarian tumor cells; and lung tumor cells.

Boyden Chamber Cell Migration Assay. Cells (5×10^4) suspended in starvation medium were added to the upper chamber of an insert (6.5 mm diameter, 8-micrometer pore size, Becton Dickenson), and the insert was placed in a 24-well dish containing starvation medium with or without 10% FBS (Yang et al. 2005, Shan et al. 2006). When used, inhibitors were added to both chambers. Migration assays were carried out for 4~6 hours and cells were fixed with 3.7% formaldehyde. Cells were stained with crystal violet staining solution, and cells on the upper side of the insert were removed with a cotton swab. Three randomly selected fields (10 x objectives) on the lower side of the insert were photographed, and the migrated cells were counted. The migration was expressed as either the average number of migrated cells in a field or as percentage of migrated cells in positive control. Percentage was calculated with the formula $P = 100 \times (M\text{-}M_{nc})/M_{pc}$, where P is the percentage of migrated cells, M is the number of migrated cells, M_{nc} is the number of migrated cells in negative controls, and M_{pc} is the number of migrated cells in positive controls.

Results

The highly invasive tumor cell lines 4T1 mouse mammary tumor cells and MDA-MB-231 human breast tumor cells were used to test the effect of decreasing fascin protein levels in tumor cells. Two different siRNAs against mouse fascin-1 and one control siRNA were used to treat 4T1 cells and cells stably expressing these siRNAs were selected. While fascin siRNAs knocked down the fascin protein levels, the control siRNA did not (FIG. 7A). Fascin siRNA-treated cells grew at comparable rates as control siRNA-treated cells and non-transfected 4T1 cells in full growth medium (data not shown), suggesting fascin is not required for breast tumor cell proliferation *in vitro*. This is consistent with previous observations that migrastatin analogs had no obvious effect on tumor cell proliferation and primary tumor growth in mouse models (Shan et al. 2005). Boyden chamber cell migration assays showed that fascin siRNA treatments, but not treatment with the control siRNA, decreased the serum-induced migration of 4T1 cells (FIG. 7B). This inhibitory effect of fascin siRNA could be rescued by transfection of human fascin cDNA (there are two nucleotide changes without amino acid changes in this specific region) (FIG. 7C and 7D). Similarly, fascin siRNA treatments down-regulated the fascin protein level and decreased the migration of MDA-MB-231 cells (FIG. 7E and 7F). Fascin siRNA treatment did not affect the proliferation of MDA-MB-231 cells (data not shown). In addition to these loss-of-function analyses, gain-of-function experiments were also performed. Comparing to metastatic MDA-MB-231 human breast tumor cells, MCF-10A normal mammary gland epithelial cells expressed less amount of fascin proteins (FIG. 7G). Overexpression of fascin in MCF-10A cells increased the serum-induced migration of these cells (FIG. 7H). Together, these data demonstrate that fascin plays a critical role in the migration of breast tumor cells.

We have solved the X-ray crystal structure of the complex of fascin and macroketone (see Example 9). Based on the structure of the complex, His474 in human fascin is essential for the macroketone binding, but not for actin-bundling. Furthermore, His474 is not conserved in Drosophila fascin, and Drosophila fascin could rescue the migration defect in 4T1 cells treated with fascin siRNAs with no sensitivity to macroketone (data not shown). As shown in FIG. 7I, while expression of human fascin in fascin siRNA-treated mouse 4T1 cells rescued the migration, this rescue was sensitive

to macroketone. In contrast, mutations of His474 to either Lys (Drosophila fascin has a Lys in the corresponding position) or Ala in human fascin rescued the migration of 4T1 cells treated with fascin siRNAs (FIG. 7I). These rescues were not inhibited by macroketone. Additionally, rescue experiments of fascin-siRNA-treated 4T1 cells with villin, another actin-bundling protein, were performed. From Drosophila genetic studies, villin partially rescued the phenotypes of fascin mutations during *Drosophila* oogenesis (Cant et al. 1996). Villin did not bind macroketone in vitro, and over-expression of villin in fascin-siRNA treated 4T1 cells partially rescued the migration which was insensitive to macroketone (data not shown). These results further confirm that fascin is the protein target for macroketone in its inhibition of tumor cell migration.

Example 7

Inhibition of fascin blocks breast tumor metastasis in mouse models

Methods

Breast Tumor Metastasis in Mice. All animal work was performed in compliance with the Institutional Animal Care and Use Committee of the Weill Medical College. Spontaneous 4T1 mouse breast tumor metastasis assay was done as described previously (Shan et al. 2005). NOD-SCID immunodeficient mice were used for experimental lung metastasis experiments. MDA-MB-231 human breast tumor cells expressing the TGL reporter were trypsinized and washed with PBS. This artificial TGL reporter gene encodes a triple fusion protein with herpes simplex virus 1 thymidine kinase fused to the N-terminus of enhanced GFP and firefly luciferase fused to the C-terminus of GFP (Ponomarev et al. 2004). Subsequently $1x10^6$ cells in 0.2 ml PBS were injected into the lateral tail vein. Luciferase-based, noninvasive bioluminescent imaging and analysis were performed with an IVIS Imaging System (Xenogen).

Cell Invasion Assay. Cells (1×10^5) suspended in starvation medium were added to the upper chamber of a Matrigel-coated insert (6.5 mm diameter, 8-μm pore size, Becton Dickenson), and the insert was placed in a 24-well dish containing medium with or without serum. When used, inhibitors were added to both chambers. Invasion assays were carried out for 16 hours and cells were fixed with 3.7% formaldehyde. Cells were stained with crystal violet staining solution, and cells on the upper side of the insert were

removed with a cotton swab. Three randomly selected fields (10 × objectives) on the lower side of the insert were photographed, and the cells on the lower surface of the insert were counted.

Results

The role of fascin in tumor metastasis was tested in animal models. The spontaneous metastasis model (with 4T1 tumor cells) and the experimental metastasis model (with MDA-MB-231 tumor cells) were used. First, it was examined whether suppression of fascin inhibits tumor invasion through a 3D matrix. As shown in FIG. 8A, expression of two fascin siRNAs in 4T1 cells dramatically reduced the 4T1 tumor cell invasion. Similarly, suppression of fascin by siRNAs in human MDA-MB-231 breast tumor cells inhibited cell invasion (data not shown). Second, the spontaneous metastasis model with 4T1 tumor cells was used to investigate the role of fascin in tumor metastasis (FIG. 8 B-D). 4T1 cells were injected into mouse mammary glands. Primary tumors from both fascin siRNA-treated cells and control siRNA-treated cells developed at similar rates (FIG. 8B) and had similar weights four weeks later (FIG. 8C), confirming that suppression of fascin did not affect proliferation of 4T1 cells *in vivo*. Four weeks after transplantation of 4T1 tumor cells, mice were sacrificed and examined for tumor metastasis to the lung (FIG. 8D). While mice injected with control siRNA-treated cells showed large numbers of metastasized 4T1 cells in the lung, fascin siRNA-treated cells failed to metastasize to the lung (FIG. 8D).

Third, the experimental metastasis model with MDA-MB-231 human tumor cells in immunodeficient mice was used to investigate the role of fascin in tumor metastasis and the effect of macroketone on the metastasis of human tumors in mice (FIG. 8 E-H). MDA-MB-231 cells were retrovirally infected with a triple-fusion protein reporter construct encoding herpes simplex virus thymidine kinase 1, green fluorescent protein (GFP) and firefly luciferase (TGL) (Minn et al. 2005). GFP-positive cells were enriched by fluorescence-activated cell sorting. These cells were injected into the tail vein of immunodeficient mice [NOD-SCID mice]. The metastasis of tumor cells to the lung was monitored by non-invasive bioluminescence imaging (Minn et al. 2005).

Most of these tumor cells became trapped in the capillaries of the lungs shortly after injection (due to size restrictions imposed by mouse capillaries, human tumor cells

are rarely able to pass from the arterial to the venous system (or vice versa) by way of the lung (Minn et al. 2005) (FIG. 8E, Day 0). A substantial attenuation of bioluminescence signal was observed within the first few days, indicating that cells that failed to metastasize were not able to survive (FIG. 8E and 8F). Progressively increasing signals after two weeks in mice with control shRNA-treated (stably expressing siRNA) tumor cells indicated that cells had succeeded in metastasizing and proliferating (FIG. 8E and 8F). Strikingly, the presence of fascin shRNA treated cells (stably expressing siRNAs) in the lung was much less than control shRNA-treated cells (FIG. 8E and 8F). Therefore, fascin siRNA treatments significantly inhibited breast tumor metastasis.

To further confirm the inhibition of tumor metastasis, histological analyses of the lung tissues from xenografted mice were performed (FIG. 8G). Lung tissues from xenografted mice were isolated and sectioned. Hematoxylin and eosin (H&E) staining showed normal structure of the lungs from mice injected with fascin siRNA-treated MDA-MB-231 tumor cells (FIG. 8G). In contrast, lung tissues from mice injected with control shRNA-treated tumor cells were heavily infiltrated by metastasized human breast tumor cells (FIG. 8G). The identity of tumor cells in the lung tissue was confirmed by GFP fluorescence since the injected MDA-MB-231 tumor cells were labeled with GFP (FIG. 8G). These results demonstrate that fascin is critical for human tumor metastasis in a mouse model.

Furthermore, it was demonstrated here that macroketone could effectively block the metastasis of human breast tumors in an animal model. The NOD-SCID mice were injected with MDA-MB-231 tumor cells with the triple-fusion protein reporter. Macroketone (10 mg/kg) or the control saline (PBS) was administered (via I.P.) on every other day for seven weeks. The effect of macroketone on the metastasis of human breast tumor cells to the lung was monitored using LivingImage software (Xenogen) by measurement of photon flux. As shown in FIG. 8H, macroketone reduced the metastasis of MDA-MB-231 cells by >80%. Together, the data demonstrate an essential role for fascin in breast tumor metastasis, and the feasibility of using the inhibitors of fascin (such as macroketone and siRNAs) as therapeutic agents for treating metastatic breast tumors.

Example 8

Elevated Expression of Fascin in Human Breast Cancer Patients

Methods

Microarray Gene Expression Analysis. Gene expression data for fascin was extracted from each tumor sample and mean-centered across all samples for each. Tissues from primary breast cancers were obtained from therapeutic procedures performed as part of routine clinical management at Memorial Sloan-Kettering Cancer Center. All research procedures using human tissue were approved by the MSKCC institutional review board (Doane et al. 2006). Tissues were snap-frozen in liquid nitrogen and stored at -80°C. Each sample was examined histologically using hemotoxylin- and eosin-stained cryostat sections. Regions were manually dissected from the frozen block to provide a consistent tumor cell content of more than 70% in tissues used for analysis. Total RNA was extracted from frozen tissue by homogenization in guanidinium isothiocyanate-based buffer (Trizol; Invitrogen, Carlsbad, CA), purified using RNAeasy (Qiagen, Valencia, CA) and examined for quality using denaturing agarose gel. Complementary DNA was synthesized from RNA using a T7-promoter-tagged oligo-dT primer. RNA target was synthesized from cDNA by in vitro transcription, and labeled with biotinylated nucleotides (Enzo Biochem, Farmingdale, NY). Gene expression analysis was performed using HG-U133A and U133B oligonucleotide microarrays according to the manufacturer's instructions (Affymetrix, Santa Clara, CA). To identify the differential gene expression, two different measures were used: fold change (ratio) between the normalized means of each group of samples and a Student's t-test.

Results

Fascin expression levels in tumor samples from human breast cancer patients were examined. A microarray gene expression data set from 137 breast cancer samples and 16 normal breast samples was analyzed. Breast tumor samples showed elevated fascin expressions comparing to normal samples (FIG. 9A). Moreover, a significant high level of fascin transcripts in the Estrogen Receptor (ER)-negative group of patients (FIG. 9B) and Progesterone Receptor (PR)-negative group of patients (FIG. 9C) was observed. Immunohistology staining with anti-fascin antibody confirmed that fascin protein was up regulated in ER-negative tumors (FIG. 9D), while ER-positive tumor cells were negative

for fascin staining (note that endothelia of vessels are fascin positive). These data reveal that fascin transcripts and protein levels are significantly elevated in aggressive ER-negative breast tumors.

Fascin mRNA expression levels in the Rosetta microarray data set of 295 breast cancer patients was also analyzed (van de Vijver et al. 2002, van 't Veer et al. 2002). Similarly, levels of fascin transcripts were significantly higher in ER-negative (FIG. 9G) and PR-negative (FIG. 9H) tumors. The Rosetta data set contains detailed clinical follow-up information of breast cancer patients. Thus, the clinical and pathological associations of fascin expression in breast cancer patients was evaluated. Kaplan-Meier analyses showed that higher fascin expression was associated with lower overall survival (FIG. 9E) and lower metastasis-free survival (FIG. 9F). These data highlight the correlation between higher fascin expression and metastasis and death in human breast cancer patients.

Example 9

Structural Basis for the Inhibition of Fascin Function and Tumor Metastasis by Migrastatin Analogs

The X-ray crystal structures of fascin in the absence and in the presence of a migrastatin analog were determined. Migrastatin analogs bind to fascin in a groove that has been biochemically and genetically defined as the surface for actin binding. These structural data provide a molecular basis for the inhibition of fascin by migrastatin analogs.

Methods

Human fascin-1 expression and purification. Recombinant human fascin-1 was expressed as GST-fusion protein in *E. coli.* Typically, a 1 liter 2YT medium with antibiotic was inoculated with 3ml overnight BL21 culture transformed with pGEX4T-Fascin1 plasmid and grown at 37°C until OD_{600} reached ~0.8. The culture was then transferred to 22 °C and 0.1mM IPTG was added for induction. After overnight induction, the bacteria were harvested by centrifugation at 5,000rpm for 10min. The bacteria pellet was snap frozen with liquid nitrogen and suspended in 30ml 1xPBS supplemented with 0.2mM PMSF, 1mM DTT, 1% Triton X-100 and 1mM EDTA. After

sonication, the suspension was centrifuged at 15,000 rpm for 60 min to remove the cell debris. The supernatant was then incubated with 4ml glutathione beads (Sigma) at 4 °C for 2 hours. After extensive wash with PBS, the beads were resuspended in 10ml thrombin cleavage buffer (20mM Tris, pH8.0, 150mM NaCl, 2mM $CaCl_2$, 1mM DTT). Human Fascin-1 was released from the beads by incubating with 40-100 units of thrombin overnight at 4°C. After centrifugation, 0.2mM PMSF was added to the supernatant to inactivate the remnant thrombin activity. The fascin protein was further purified with a Superdex 200 gel filtration column and concentrated with Centricon to about 80mg/ml. The typical yield from a 1 liter culture is about 40mg.

Crystalization and structure determination. Concentrated fascin stock was diluted with fascin buffer (20mM Tris, pH8.0, 40mM KBr, 0.5mM EDTA, 1mM DTT) to 15mg/ml. For the growth of fascin-macroketone complex, the protein was incubated with 2mM macroketone at room temperature for 1 hour. The crystal drops were set up by hanging drop diffusion at 20°C in reservoir solution that contained 100mM Hepes, pH8.0, 16% PEG4000, 1% isopropanol. Crystals were harvest in cryo-solution (100mM Hepes, pH8.0, 16% PEG400, 15% glycerol) and snap frozen in liquid nitrogen. X-ray diffraction data were collected from frozen crystals at National Synchrotron Light Source beamline X6a at Brookhaven National Laboratory. The atomic models of fascin and fascin-macroketone complex were initially obtained by molecular replacement with 1dfc model using Phaser. The structures were manually adjusted with Coot and refined with CNS and Refmac5 with R_{free} sets containing 5% of the reflections. Two fascin molecules were found in each asymmetric unit.

Actin bundling assay. The actin bundling assay was performed as described in Example 4 above.

Results

Overall Structure and Topology of Human Fascin-1. The X-ray crystal structure of native human fascin-1 as well as fascin-1 in complex with a migrastatin analog, the macroketone core, was determined (FIG. 10A, B and C). Both crystals belong to C2 space group. The native fascin structure and the structure of fascin-macroketone complex was determined at 2.1 Å and 2.7 Å, respectively (FIG. 10 A, B and C). The overall structure of fascin exhibits four β-trefoil folds, with β-trefoil 1 and 2 forming a

dumbbell-shaped domain, and β-trefoil 3 and 4 forming another (FIG.10A). The two dumbbells are inter-connected by a loop between β-trefoil 2 and 3. The two dumbbell domains are arranged in a way that trefoil 2 directly contacts trefoil 3 and 4, while trefoil 4 directly contacts trefoil 1 and 2 (FIG.10A). Overall, the two dumbbells create a horseshoe appearance.

Migrastatin Analog Binding Pocket. The overall domain arrangement of fascin-macroketone complex is very similar to that of the native fascin, with two dumbbells forming the two arms of a horseshoe (FIG. 10C). A 3σ F_{obs}-F_{calc} electron density peak was observed on the surface of β-trefoil 4 (FIG. 11A). The macrolide ring of macroketone fits well with the extra density. The bound macroketone molecule sits at the surface of trefoil 4, on the side facing the cleft between trefoil 4 and trefoil 1 (FIG. 10C). Macroketone is held in place by interacting with the side chains of His392, Glu391, Ala488, Lys471, and His474 as well as the alpha carbon of Asp473 (FIG. 11 A–D). The six residues form a U-shape curvature, holding macroketone like holding a ring with thumb and index finger (FIG. 11A and 11B). On the top of the two "fingers" are the two histidines, His392 and His474, which have major contributions to the fascin-macroketone interaction. The NE2 nitrogen of His392 is 3.01 Å away from the ketone oxygen of macroketone molecule, while the ND1 nitrogen of His474 is 2.57 Å away from the hydroxyl oxygen. His392 and His474 contribute to the binding of macroketone by forming hydrogen bonds with macroketone (FIG. 11B). The interaction between fascin and macroketone is further stabilized by the *van der Waals* force between the macrolide ring carbon and residue Glu391, Ala488, Lys471 and Asp473 (FIG. 11B).

Although the overall structure of fascin-macroketone complex is similar to the native fascin, with a root mean square deviation (RMSD) of 0.3 Å for all the alpha carbon atoms (FIG. 11C), several residues at the "thumb-and-index-finger" binding site for macroketone move as a result of "induced-fit" mechanism (FIG. 11D). While the alpha Cα of His474 moves about 2 Å away from the macroketone, its imidazole group is rotated by 180° about its Cα-Cβ bond toward the molecule. Consequently, the ND1 nitrogen of His474 moves 2.3 Å closer to form hydrogen bond with the hydroxyl group of macroketone. Meanwhile, the imidazole group of His392, which forms hydrogen bond with the ketone group of macroketone, is pushed 1Å away. The carboxyl group of

Asp473 also rotates 90° about its Cβ-Cγ bound as a consequence of the inhibitor-fascin interaction.

Actin binding sites. Fascin functions as a monomer to bundle actin filaments, and it has been proposed that fascin has two actin-binding sites for this bundling activity (Ono et al. 1997). The crystal structure shown herein provides a structural explanation for this (FIG. 12A and 12B, orange and cyan labeled residues). Both the N-and C-termini are located in the same cleft (FIG. 12A and 12B). Furthermore, a stretch of residues from 29 to 42 at the N-terminal, which has similarity to an actin binding site of MARCKS (myristoylated alanine-rich C-kinase substrate), is also facing the trefoil 1- 4 cleft (FIG. 12C, orange labeled residues in the original). Moreover, the actin bundling activity of fascin is negatively regulated by a protein kinase C phosphorylation site (Ser39) within the N-terminal region (FIG. 12D, the red labeled residue in the original). Together, these data suggest that this cleft represents one of the two actin-binding sites.

Genetic analysis of the Drosophila fascin homolog, singed, yielded two point mutations of fascin which are critical for its actin bundling activity (Cant et al. 1996). One mutation is Gly393 (Gly409 in *Drosophila*) to Glu that reduced the actin-bundling activity of fascin (FIG. 12D, the red label residue). This Gly393 locates in the above-mentioned actin binding site. On the other hand, another *singed* mutant is Ser274 (Ser289 in *Drosophila*) to Asn that almost eliminated the actin-bundling activity of fascin (FIG. 12E). This Ser274 locates on the opposite side of fascin (FIG. 12E). This surface may represent the second actin-binding site.

Biochemical and structural studies of the interaction of F-actin filaments and fimbrin, another actin bundling protein revealed two actin-binding sites. These two actin-binding sites on fimbrin are located in similar surfaces as the two potential actin-binding sites of fascin. Even though fimbrin consists of entirely α-helical structures and fascin with all β-sheets, they have similar overall structural arrangements.

Macroketone binds to one of the actin binding sites on fascin. The structure of the fascin-macroketone complex immediately suggested a possible mechanism by which macroketone inhibits the actin bundling activity of fascin. The macroketone binding site is one of the actin binding sites on fascin (FIG. 13A). Therefore, although not being

bound by any specific theory, it appears that macroketone binding interferes with the binding of actin filament binding to fascin (FIG. 13B).

Five residues involved in macroketone binding were mutated and the actin bundling activity of those fascin mutants was examined (FIG. 14). Based on the actin bundling assays, His392, Lys471 and Ala488 are critical for actin bundling, while Glu391 and His474 are not (FIG. 14A and 14B). Furthermore, the sensitivity of the actin bundling activity of Glu391 and His474 to macroketone was examined (mutants His392, Lys471 and Ala488 were not tested due to their defective actin bundling activity). As shown in FIG. 14C, mutation of His474 to Ala rendered fascin to resistant to macroketone treatment. Therefore, His474 is essential for macroketone binding. Taken together, this data demonstrates that several fascin residues involved in macroketone binding also contribute to actin binding. Hence, the macroketone binding site is one of the actin binding sites.

Table 2: Atomic Coordinates for Fascin

```
REMARK coordinates from water picking
REMARK 59 waters picked at level greater than 3.0
REMARK in (1 m|Fo| - 1 D|Fc|)e^(i phi_calc) cross-val. sigmaa map
REMARK peak selection criteria: hbond
REMARK peaks closer than 2.6 A or further than 4.0 A were deleted
REMARK but peaks 2.0 A from oxygen or nitrogen were kept
REMARK peaks further than 3.2 A from a oxygen or nitrogen were deleted
REMARK map resolution: 30 - 2.7 A
REMARK starting r= 0.2707 free_r= 0.2898
REMARK final    r= 0.2666 free_r= 0.2874
REMARK sg=C2 a=160.358 b=70.407 c=112.398 alpha=90 beta=131.890
gamma=90
REMARK parameter file 1  : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2  : CNS_TOPPAR:dna-rna_rep.param
REMARK parameter file 3  : CNS_TOPPAR:water_rep.param
REMARK parameter file 4  : CNS_TOPPAR:ion.param
REMARK parameter file 5  : ../xyz.param
REMARK molecular structure file: ../gen_xyz.mtf
REMARK input coordinates: ../gen_xyz.pdb
REMARK anomalous f' f'' library: CNS_XRAYLIB:anom_cu.lib
REMARK reflection file= ../../070919.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 2.7
REMARK initial B-factor correction applied to fobs :
REMARK   B11=  -5.627 B22=  16.015 B33= -10.388
REMARK   B12=   0.000 B13= -17.572 B23=   0.000
REMARK B-factor correction applied to coordinate array B:    0.103
REMARK bulk solvent: density level= 0.262554 e/A^3, B-factor= 50.3504
A^2
```

```
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 25837(100.0%)
REMARK number unobserved reflections (no entry or |F|=0):  1298 (5.0%)
REMARK number reflections rejected:                           0 (0.0%)
REMARK total number of reflections used:                  24539 (95.0%)
REMARK number of reflections in working set:              23345 (90.4%)
REMARK number of reflections in test set:                  1194 (4.6%)
CRYST1  160.358   70.407  112.398  90.00 131.89  90.00 C 2
REMARK FILENAME="wat_keton.pdb"
REMARK VERSION:1.1

  Atom   Amino Acid
  1  C   GLY A1005   -31.443  -4.644  38.038  1.00 63.56    A
  2  O   GLY A1005   -32.038  -3.530  38.056  1.00 62.44    A
  3  N   GLY A1005   -29.088  -5.801  37.808  1.00 56.65    A
  4  CA  GLY A1005   -29.928  -4.728  38.385  1.00 60.77    A
  5  N   THR A1006   -32.092  -5.782  37.702  1.00 65.25    A
  6  CA  THR A1006   -33.445  -5.702  37.031  1.00 65.48    A
  7  CB  THR A1006   -34.439  -5.824  38.145  1.00 65.56    A
  8  OG1 THR A1006   -33.942  -4.955  39.157  1.00 68.68    A
  9  CG2 THR A1006   -34.358  -7.219  38.631  1.00 64.18    A
 10  C   THR A1006   -33.760  -4.410  36.107  1.00 64.13    A
 11  O   THR A1006   -34.699  -3.708  36.296  1.00 62.77    A
 12  N   ALA A1007   -32.966  -4.151  35.080  1.00 64.41    A
 13  CA  ALA A1007   -32.720  -2.714  34.527  1.00 63.53    A
 14  CB  ALA A1007   -33.362  -1.508  35.354  1.00 60.50    A
 15  C   ALA A1007   -31.234  -2.448  34.187  1.00 61.16    A
 16  O   ALA A1007   -30.964  -1.986  33.050  1.00 62.88    A
 17  N   GLU A1008   -30.320  -2.906  35.035  1.00 56.50    A
 18  CA  GLU A1008   -28.925  -2.599  35.003  1.00 57.05    A
 19  CB  GLU A1008   -28.186  -3.748  34.434  1.00 57.04    A
 20  CG  GLU A1008   -28.631  -4.104  32.945  1.00 65.47    A
 21  CD  GLU A1008   -27.582  -4.861  32.133  1.00 61.58    A
 22  OE1 GLU A1008   -27.882  -5.875  31.423  1.00 57.53    A
 23  OE2 GLU A1008   -26.439  -4.360  32.233  1.00 68.27    A
 24  C   GLU A1008   -28.470  -1.263  34.370  1.00 57.18    A
 25  O   GLU A1008   -27.819  -1.227  33.302  1.00 59.63    A
 26  N   ALA A1009   -28.775  -0.132  34.995  1.00 55.46    A
 27  CA  ALA A1009   -28.384   1.140  34.402  1.00 54.55    A
 28  CB  ALA A1009   -29.029   2.248  35.181  1.00 54.39    A
 29  C   ALA A1009   -26.855   1.395  34.317  1.00 54.99    A
 30  O   ALA A1009   -26.047   0.785  35.022  1.00 56.25    A
 31  N   VAL A1010   -26.443   2.365  33.526  1.00 52.26    A
 32  CA  VAL A1010   -25.062   2.642  33.504  1.00 48.76    A
 33  CB  VAL A1010   -24.714   3.185  32.068  1.00 47.46    A
 34  CG1 VAL A1010   -25.535   4.409  31.877  1.00 51.64    A
 35  CG2 VAL A1010   -23.307   3.638  31.932  1.00 44.47    A
 36  C   VAL A1010   -24.654   3.566  34.725  1.00 49.13    A
 37  O   VAL A1010   -25.368   4.455  35.313  1.00 47.71    A
 38  N   GLN A1011   -23.423   3.380  35.086  1.00 48.76    A
 39  CA  GLN A1011   -22.969   4.026  36.226  1.00 48.93    A
 40  CB  GLN A1011   -22.387   3.046  37.343  1.00 47.97    A
 41  CG  GLN A1011   -21.624   3.899  38.409  1.00 50.69    A
 42  CD  GLN A1011   -20.686   3.136  39.306  1.00 52.22    A
 43  OE1 GLN A1011   -19.537   3.027  38.983  1.00 52.51    A
```

44	NE2	GLN	A1011	-21.182	2.581	40.455	1.00	56.23	A
45	C	GLN	A1011	-21.974	4.891	35.592	1.00	45.39	A
46	O	GLN	A1011	-20.977	4.392	35.155	1.00	45.78	A
47	N	ILE	A1012	-22.259	6.202	35.656	1.00	45.34	A
48	CA	ILE	A1012	-21.454	7.310	35.208	1.00	42.98	A
49	CB	ILE	A1012	-22.198	8.623	35.253	1.00	43.06	A
50	CG2	ILE	A1012	-21.435	9.629	34.467	1.00	39.58	A
51	CG1	ILE	A1012	-23.537	8.635	34.563	1.00	44.21	A
52	CD1	ILE	A1012	-23.898	7.513	33.615	1.00	47.82	A
53	C	ILE	A1012	-20.283	7.466	36.121	1.00	44.47	A
54	O	ILE	A1012	-20.437	7.549	37.331	1.00	43.06	A
55	N	GLN	A1013	-19.144	7.534	35.470	1.00	45.23	A
56	CA	GLN	A1013	-17.860	7.721	35.934	1.00	48.94	A
57	CB	GLN	A1013	-17.030	6.407	35.828	1.00	51.51	A
58	CG	GLN	A1013	-17.399	5.553	37.087	1.00	51.83	A
59	CD	GLN	A1013	-16.392	4.558	37.594	1.00	50.69	A
60	OE1	GLN	A1013	-15.797	3.768	36.837	1.00	57.64	A
61	NE2	GLN	A1013	-16.242	4.525	38.929	1.00	53.80	A
62	C	GLN	A1013	-17.261	8.769	35.059	1.00	51.14	A
63	O	GLN	A1013	-17.304	8.672	33.836	1.00	54.16	A
64	N	PHE	A1014	-16.661	9.798	35.666	1.00	54.55	A
65	CA	PHE	A1014	-15.954	10.855	34.881	1.00	52.56	A
66	CB	PHE	A1014	-16.895	11.801	34.338	1.00	50.01	A
67	CG	PHE	A1014	-17.703	12.476	35.300	1.00	48.05	A
68	CD1	PHE	A1014	-17.238	13.529	35.997	1.00	46.54	A
69	CD2	PHE	A1014	-18.984	12.161	35.457	1.00	47.73	A
70	CE1	PHE	A1014	-18.106	14.281	36.835	1.00	44.30	A
71	CE2	PHE	A1014	-19.838	12.871	36.354	1.00	47.96	A
72	CZ	PHE	A1014	-19.379	13.929	37.031	1.00	46.03	A
73	C	PHE	A1014	-14.757	11.540	35.451	1.00	53.11	A
74	O	PHE	A1014	-14.515	11.602	36.605	1.00	54.55	A
75	N	GLY	A1015	-13.918	11.979	34.587	1.00	53.94	A
76	CA	GLY	A1015	-12.948	13.012	35.018	1.00	54.68	A
77	C	GLY	A1015	-13.478	14.427	34.870	1.00	54.65	A
78	O	GLY	A1015	-14.241	14.800	33.871	1.00	55.71	A
79	N	LEU	A1016	-13.113	15.260	35.832	1.00	54.35	A
80	CA	LEU	A1016	-13.655	16.708	35.822	1.00	55.52	A
81	CB	LEU	A1016	-14.531	16.970	36.986	1.00	54.00	A
82	CG	LEU	A1016	-15.879	17.697	36.981	1.00	54.40	A
83	CD1	LEU	A1016	-16.686	17.585	35.673	1.00	59.29	A
84	CD2	LEU	A1016	-16.625	17.246	38.252	1.00	49.57	A
85	C	LEU	A1016	-12.480	17.679	35.737	1.00	55.53	A
86	O	LEU	A1016	-11.480	17.411	36.361	1.00	54.23	A
87	N	ILE	A1017	-12.554	18.622	34.780	1.00	57.79	A
88	CA	ILE	A1017	-11.364	19.364	34.146	1.00	60.86	A
89	CB	ILE	A1017	-11.268	19.112	32.589	1.00	62.78	A
90	CG2	ILE	A1017	-10.082	19.879	31.923	1.00	59.65	A
91	CG1	ILE	A1017	-10.985	17.633	32.267	1.00	63.94	A
92	CD1	ILE	A1017	-11.025	17.347	30.631	1.00	63.88	A
93	C	ILE	A1017	-11.385	20.908	34.261	1.00	58.77	A
94	O	ILE	A1017	-12.198	21.546	33.673	1.00	55.86	A
95	N	ASN	A1018	-10.472	21.444	35.058	1.00	59.04	A
96	CA	ASN	A1018	-10.460	22.895	35.499	1.00	58.78	A
97	CB	ASN	A1018	-10.271	23.020	37.084	1.00	57.34	A
98	CG	ASN	A1018	-8.905	23.615	37.519	1.00	53.04	A
99	OD1	ASN	A1018	-7.796	23.066	37.248	1.00	44.38	A

100	ND2	ASN	A1018	-8.989	24.776	38.180	1.00	50.40	A
101	C	ASN	A1018	-9.431	23.838	34.892	1.00	59.06	A
102	O	ASN	A1018	-8.240	23.409	34.404	1.00	58.09	A
103	N	CYS	A1019	-9.816	25.098	35.153	1.00	57.40	A
104	CA	CYS	A1019	-8.958	26.299	34.922	1.00	57.47	A
105	CB	CYS	A1019	-8.570	26.929	36.237	1.00	57.44	A
106	SG	CYS	A1019	-9.436	28.406	36.579	1.00	64.67	A
107	C	CYS	A1019	-7.740	25.864	34.224	1.00	53.98	A
108	O	CYS	A1019	-7.850	25.354	33.207	1.00	55.20	A
109	N	GLY	A1020	-6.593	26.003	34.798	1.00	52.78	A
110	CA	GLY	A1020	-5.395	25.267	34.338	1.00	54.49	A
111	C	GLY	A1020	-5.401	23.751	33.866	1.00	52.79	A
112	O	GLY	A1020	-4.440	23.061	34.077	1.00	49.42	A
113	N	ASN	A1021	-6.421	23.274	33.161	1.00	53.56	A
114	CA	ASN	A1021	-6.248	21.945	32.548	1.00	57.24	A
115	CB	ASN	A1021	-5.281	21.939	31.283	1.00	57.08	A
116	CG	ASN	A1021	-5.988	21.633	29.826	1.00	51.13	A
117	OD1	ASN	A1021	-5.309	21.269	28.861	1.00	51.04	A
118	ND2	ASN	A1021	-7.249	21.809	29.706	1.00	42.97	A
119	C	ASN	A1021	-5.561	21.096	33.734	1.00	59.54	A
120	O	ASN	A1021	-4.461	20.385	33.460	1.00	59.25	A
121	N	LYS	A1022	-6.123	21.237	34.999	1.00	56.29	A
122	CA	LYS	A1022	-5.871	20.258	36.031	1.00	52.35	A
123	CB	LYS	A1022	-5.330	20.966	37.254	1.00	50.78	A
124	CG	LYS	A1022	-3.985	21.344	37.117	1.00	43.26	A
125	CD	LYS	A1022	-3.055	20.215	36.580	1.00	40.80	A
126	CE	LYS	A1022	-1.568	20.479	36.850	1.00	31.19	A
127	NZ	LYS	A1022	-0.689	20.298	35.669	1.00	44.88	A
128	C	LYS	A1022	-7.182	19.503	36.385	1.00	54.00	A
129	O	LYS	A1022	-8.242	20.122	36.575	1.00	56.17	A
130	N	TYR	A1023	-7.149	18.176	36.447	1.00	53.84	A
131	CA	TYR	A1023	-8.370	17.376	36.798	1.00	53.31	A
132	CB	TYR	A1023	-8.031	15.899	36.552	1.00	52.89	A
133	CG	TYR	A1023	-8.144	15.497	35.188	1.00	50.27	A
134	CD1	TYR	A1023	-7.085	15.373	34.422	1.00	56.94	A
135	CE1	TYR	A1023	-7.203	15.011	33.082	1.00	58.64	A
136	CD2	TYR	A1023	-9.369	15.271	34.626	1.00	51.76	A
137	CE2	TYR	A1023	-9.512	14.955	33.319	1.00	48.09	A
138	CZ	TYR	A1023	-8.425	14.786	32.552	1.00	55.01	A
139	OH	TYR	A1023	-8.562	14.364	31.215	1.00	55.49	A
140	C	TYR	A1023	-8.718	17.482	38.298	1.00	52.99	A
141	O	TYR	A1023	-7.860	17.564	39.098	1.00	54.53	A
142	N	LEU	A1024	-9.938	17.272	38.650	1.00	52.04	A
143	CA	LEU	A1024	-10.379	17.200	40.023	1.00	53.31	A
144	CB	LEU	A1024	-11.920	17.015	39.977	1.00	52.76	A
145	CG	LEU	A1024	-12.669	17.757	41.065	1.00	53.91	A
146	CD1	LEU	A1024	-14.036	17.164	41.086	1.00	43.01	A
147	CD2	LEU	A1024	-11.902	17.825	42.609	1.00	51.84	A
148	C	LEU	A1024	-9.753	16.080	40.891	1.00	52.85	A
149	O	LEU	A1024	-9.661	14.948	40.447	1.00	56.13	A
150	N	THR	A1025	-9.332	16.319	42.125	1.00	52.61	A
151	CA	THR	A1025	-8.397	15.249	42.730	1.00	52.97	A
152	CB	THR	A1025	-7.044	15.367	42.179	1.00	50.65	A
153	OG1	THR	A1025	-7.278	15.190	40.852	1.00	52.08	A
154	CG2	THR	A1025	-6.170	14.310	42.559	1.00	47.81	A
155	C	THR	A1025	-8.395	14.877	44.248	1.00	54.00	A

ATOM	156	O	THR	A1025	-8.002	15.670	45.098	1.00 52.19	A
ATOM	157	N	ALA	A1026	-8.894	13.675	44.552	1.00 54.51	A
ATOM	158	CA	ALA	A1026	-8.824	13.212	45.909	1.00 55.31	A
ATOM	159	CB	ALA	A1026	-10.028	12.637	46.306	1.00 53.96	A
ATOM	160	C	ALA	A1026	-7.650	12.277	46.062	1.00 55.88	A
ATOM	161	O	ALA	A1026	-7.548	11.276	45.445	1.00 57.50	A
ATOM	162	N	GLU	A1027	-6.743	12.621	46.927	1.00 55.61	A
ATOM	163	CA	GLU	A1027	-5.492	12.001	46.893	1.00 55.01	A
ATOM	164	CB	GLU	A1027	-4.478	13.044	47.260	1.00 54.55	A
ATOM	165	CG	GLU	A1027	-4.521	14.391	46.447	1.00 55.17	A
ATOM	166	CD	GLU	A1027	-3.520	14.307	45.359	1.00 55.86	A
ATOM	167	OE1	GLU	A1027	-3.154	15.269	44.596	1.00 55.85	A
ATOM	168	OE2	GLU	A1027	-3.034	13.193	45.377	1.00 55.71	A
ATOM	169	C	GLU	A1027	-5.625	11.049	48.023	1.00 57.42	A
ATOM	170	O	GLU	A1027	-6.747	10.854	48.608	1.00 55.47	A
ATOM	171	N	ALA	A1028	-4.468	10.460	48.395	1.00 57.69	A
ATOM	172	CA	ALA	A1028	-4.549	9.518	49.458	1.00 57.44	A
ATOM	173	CB	ALA	A1028	-3.610	8.317	49.175	1.00 58.00	A
ATOM	174	C	ALA	A1028	-4.284	10.175	50.861	1.00 58.03	A
ATOM	175	O	ALA	A1028	-4.102	9.419	51.865	1.00 59.82	A
ATOM	176	N	PHE	A1029	-4.209	11.517	50.881	1.00 57.48	A
ATOM	177	CA	PHE	A1029	-3.890	12.433	52.034	1.00 57.08	A
ATOM	178	CB	PHE	A1029	-3.433	13.850	51.543	1.00 59.26	A
ATOM	179	CG	PHE	A1029	-2.189	13.877	50.866	1.00 57.88	A
ATOM	180	CD1	PHE	A1029	-2.169	14.031	49.448	1.00 59.87	A
ATOM	181	CD2	PHE	A1029	-1.026	13.752	51.610	1.00 57.84	A
ATOM	182	CE1	PHE	A1029	-0.978	13.930	48.672	1.00 53.85	A
ATOM	183	CE2	PHE	A1029	0.201	13.720	50.953	1.00 67.06	A
ATOM	184	CZ	PHE	A1029	0.243	13.854	49.433	1.00 65.71	A
ATOM	185	C	PHE	A1029	-5.161	12.861	52.684	1.00 55.47	A
ATOM	186	O	PHE	A1029	-6.147	13.143	51.957	1.00 56.57	A
ATOM	187	N	GLY	A1030	-5.137	12.979	53.978	1.00 50.11	A
ATOM	188	CA	GLY	A1030	-5.988	13.905	54.585	1.00 50.10	A
ATOM	189	C	GLY	A1030	-7.388	14.051	54.169	1.00 50.62	A
ATOM	190	O	GLY	A1030	-8.121	14.830	54.733	1.00 51.04	A
ATOM	191	N	PHE	A1031	-7.790	13.224	53.220	1.00 50.67	A
ATOM	192	CA	PHE	A1031	-8.910	13.497	52.358	1.00 50.15	A
ATOM	193	CB	PHE	A1031	-10.238	13.520	53.055	1.00 49.29	A
ATOM	194	CG	PHE	A1031	-10.476	12.283	53.875	1.00 54.80	A
ATOM	195	CD1	PHE	A1031	-11.344	12.296	54.938	1.00 55.12	A
ATOM	196	CD2	PHE	A1031	-9.774	11.051	53.572	1.00 57.41	A
ATOM	197	CE1	PHE	A1031	-11.425	11.192	55.768	1.00 60.16	A
ATOM	198	CE2	PHE	A1031	-9.905	9.964	54.376	1.00 58.47	A
ATOM	199	CZ	PHE	A1031	-10.728	10.024	55.459	1.00 57.52	A
ATOM	200	C	PHE	A1031	-8.730	14.718	51.615	1.00 51.59	A
ATOM	201	O	PHE	A1031	-9.488	15.609	51.795	1.00 51.95	A
ATOM	202	N	LYS	A1032	-7.758	14.794	50.728	1.00 53.43	A
ATOM	203	CA	LYS	A1032	-7.706	16.026	49.994	1.00 56.72	A
ATOM	204	CB	LYS	A1032	-6.341	16.682	50.093	1.00 55.47	A
ATOM	205	CG	LYS	A1032	-6.294	17.746	51.123	1.00 54.23	A
ATOM	206	CD	LYS	A1032	-5.107	17.362	52.207	1.00 55.22	A
ATOM	207	CE	LYS	A1032	-4.473	18.539	52.956	1.00 47.58	A
ATOM	208	NZ	LYS	A1032	-5.599	19.425	53.489	1.00 43.63	A
ATOM	209	C	LYS	A1032	-8.199	15.947	48.527	1.00 59.09	A
ATOM	210	O	LYS	A1032	-7.974	14.908	47.835	1.00 60.43	A
ATOM	211	N	VAL	A1033	-8.839	17.067	48.110	1.00 59.33	A

212	CA	VAL	A1033	-9.520	17.275	46.835	1.00	58.64	A
213	CB	VAL	A1033	-11.057	17.328	47.124	1.00	58.02	A
214	CG1	VAL	A1033	-11.312	18.381	48.239	1.00	59.34	A
215	CG2	VAL	A1033	-11.755	17.752	45.949	1.00	54.93	A
216	C	VAL	A1033	-8.981	18.561	46.065	1.00	58.41	A
217	O	VAL	A1033	-9.529	19.667	46.071	1.00	57.02	A
218	N	ASN	A1034	-7.908	18.373	45.332	1.00	59.46	A
219	CA	ASN	A1034	-7.249	19.515	44.700	1.00	59.67	A
220	CB	ASN	A1034	-5.731	19.495	44.859	1.00	56.12	A
221	CG	ASN	A1034	-5.135	18.242	44.369	1.00	56.34	A
222	OD1	ASN	A1034	-5.229	17.937	43.158	1.00	61.05	A
223	ND2	ASN	A1034	-4.470	17.443	45.305	1.00	51.67	A
224	C	ASN	A1034	-7.613	19.513	43.228	1.00	60.16	A
225	O	ASN	A1034	-8.550	18.798	42.809	1.00	60.76	A
226	N	ALA	A1035	-6.895	20.379	42.499	1.00	58.69	A
227	CA	ALA	A1035	-6.887	20.397	41.074	1.00	57.21	A
228	CB	ALA	A1035	-7.342	21.722	40.556	1.00	56.17	A
229	C	ALA	A1035	-5.457	20.331	40.868	1.00	57.36	A
230	O	ALA	A1035	-4.954	21.267	40.397	1.00	58.76	A
231	N	SER	A1036	-4.763	19.252	41.258	1.00	58.33	A
232	CA	SER	A1036	-3.423	19.142	40.880	1.00	56.02	A
233	CB	SER	A1036	-2.504	19.404	42.026	1.00	56.56	A
234	OG	SER	A1036	-2.294	20.862	42.070	1.00	52.28	A
235	C	SER	A1036	-2.908	18.337	39.670	1.00	57.13	A
236	O	SER	A1036	-1.727	18.556	39.257	1.00	57.60	A
237	N	ALA	A1037	-3.874	17.749	38.941	1.00	56.75	A
238	CA	ALA	A1037	-3.868	16.429	38.298	1.00	56.13	A
239	CB	ALA	A1037	-5.246	15.897	38.585	1.00	55.02	A
240	C	ALA	A1037	-3.754	16.565	36.781	1.00	57.24	A
241	O	ALA	A1037	-4.554	17.355	36.119	1.00	54.07	A
242	N	SER	A1038	-2.805	15.849	36.167	1.00	58.31	A
243	CA	SER	A1038	-2.584	16.230	34.703	1.00	59.47	A
244	CB	SER	A1038	-1.209	16.909	34.522	1.00	58.39	A
245	OG	SER	A1038	-0.144	15.988	34.401	1.00	55.29	A
246	C	SER	A1038	-2.705	15.058	33.783	1.00	59.94	A
247	O	SER	A1038	-1.792	14.792	33.072	1.00	60.52	A
248	N	SER	A1039	-3.800	14.298	33.916	1.00	60.43	A
249	CA	SER	A1039	-3.994	12.917	33.372	1.00	57.59	A
250	CB	SER	A1039	-2.801	12.043	33.700	1.00	56.68	A
251	OG	SER	A1039	-3.031	10.742	33.239	1.00	56.29	A
252	C	SER	A1039	-5.228	12.391	34.033	1.00	56.58	A
253	O	SER	A1039	-5.500	12.792	35.122	1.00	57.19	A
254	N	LEU	A1040	-6.063	11.635	33.336	1.00	57.07	A
255	CA	LEU	A1040	-7.133	10.817	34.010	1.00	56.28	A
256	CB	LEU	A1040	-8.294	10.499	33.051	1.00	55.51	A
257	CG	LEU	A1040	-9.806	10.756	33.251	1.00	52.43	A
258	CD1	LEU	A1040	-10.564	9.742	32.516	1.00	49.92	A
259	CD2	LEU	A1040	-10.291	10.778	34.711	1.00	50.34	A
260	C	LEU	A1040	-6.554	9.469	34.459	1.00	56.62	A
261	O	LEU	A1040	-6.335	8.672	33.614	1.00	55.18	A
262	N	LYS	A1041	-6.255	9.289	35.793	1.00	59.43	A
263	CA	LYS	A1041	-5.888	7.984	36.569	1.00	55.50	A
264	CB	LYS	A1041	-4.469	7.956	37.081	1.00	54.44	A
265	CG	LYS	A1041	-3.441	8.411	36.085	1.00	52.16	A
266	CD	LYS	A1041	-3.846	7.799	34.618	1.00	58.24	A
267	CE	LYS	A1041	-3.131	6.336	34.256	1.00	52.00	A

268	NZ	LYS	A1041	-3.760	5.654	33.060	1.00	49.99	A
269	C	LYS	A1041	-6.757	7.938	37.754	1.00	55.56	A
270	O	LYS	A1041	-7.710	8.676	37.842	1.00	57.31	A
271	N	LYS	A1042	-6.484	7.028	38.677	1.00	55.81	A
272	CA	LYS	A1042	-7.457	6.648	39.701	1.00	53.94	A
273	CB	LYS	A1042	-6.816	5.776	40.706	1.00	53.20	A
274	CG	LYS	A1042	-6.934	4.328	40.409	1.00	57.97	A
275	CD	LYS	A1042	-5.563	3.807	39.917	1.00	59.08	A
276	CE	LYS	A1042	-4.698	3.164	41.081	1.00	52.12	A
277	NZ	LYS	A1042	-3.345	2.820	40.751	1.00	37.82	A
278	C	LYS	A1042	-8.047	7.785	40.483	1.00	54.82	A
279	O	LYS	A1042	-9.254	7.756	40.786	1.00	57.56	A
280	N	LYS	A1043	-7.251	8.793	40.910	1.00	54.21	A
281	CA	LYS	A1043	-7.796	9.757	41.964	1.00	50.42	A
282	CB	LYS	A1043	-6.653	10.501	42.658	1.00	48.64	A
283	CG	LYS	A1043	-5.936	9.825	43.796	1.00	47.06	A
284	CD	LYS	A1043	-4.634	9.320	43.398	1.00	37.10	A
285	CE	LYS	A1043	-3.627	9.756	44.259	1.00	39.10	A
286	NZ	LYS	A1043	-2.363	10.523	43.584	1.00	39.03	A
287	C	LYS	A1043	-8.594	10.783	41.170	1.00	50.70	A
288	O	LYS	A1043	-9.137	11.768	41.750	1.00	50.11	A
289	N	GLN	A1044	-8.539	10.647	39.808	1.00	50.83	A
290	CA	GLN	A1044	-9.185	11.587	38.850	1.00	50.83	A
291	CB	GLN	A1044	-8.375	11.693	37.616	1.00	52.80	A
292	CG	GLN	A1044	-7.048	12.599	37.687	1.00	56.90	A
293	CD	GLN	A1044	-6.165	12.507	38.974	1.00	55.33	A
294	OE1	GLN	A1044	-5.494	11.531	39.255	1.00	61.26	A
295	NE2	GLN	A1044	-6.076	13.566	39.623	1.00	60.28	A
296	C	GLN	A1044	-10.616	11.184	38.493	1.00	50.18	A
297	O	GLN	A1044	-11.497	12.050	38.383	1.00	51.43	A
298	N	ILE	A1045	-10.869	9.879	38.463	1.00	49.98	A
299	CA	ILE	A1045	-12.221	9.247	38.411	1.00	50.18	A
300	CB	ILE	A1045	-12.232	7.758	37.903	1.00	48.74	A
301	CG2	ILE	A1045	-11.251	7.502	36.648	1.00	49.78	A
302	CG1	ILE	A1045	-11.726	6.852	38.879	1.00	52.23	A
303	CD1	ILE	A1045	-12.465	5.526	38.804	1.00	56.67	A
304	C	ILE	A1045	-13.155	9.494	39.607	1.00	49.28	A
305	O	ILE	A1045	-12.859	9.204	40.717	1.00	51.66	A
306	N	TRP	A1046	-14.275	10.116	39.318	1.00	49.66	A
307	CA	TRP	A1046	-15.277	10.535	40.216	1.00	50.01	A
308	CB	TRP	A1046	-15.555	12.077	40.014	1.00	49.08	A
309	CG	TRP	A1046	-14.479	12.821	40.716	1.00	47.72	A
310	CD2	TRP	A1046	-14.377	13.050	42.124	1.00	42.59	A
311	CE2	TRP	A1046	-13.068	13.513	42.385	1.00	53.93	A
312	CE3	TRP	A1046	-15.250	12.921	43.169	1.00	46.79	A
313	CD1	TRP	A1046	-13.229	13.115	40.198	1.00	49.26	A
314	NE1	TRP	A1046	-12.368	13.530	41.182	1.00	47.35	A
315	CZ2	TRP	A1046	-12.638	13.917	43.726	1.00	49.17	A
316	CZ3	TRP	A1046	-14.853	13.346	44.499	1.00	51.34	A
317	CH2	TRP	A1046	-13.581	13.864	44.740	1.00	48.93	A
318	C	TRP	A1046	-16.399	9.631	39.676	1.00	52.70	A
319	O	TRP	A1046	-16.531	9.581	38.427	1.00	54.08	A
320	N	THR	A1047	-17.122	8.887	40.560	1.00	52.16	A
321	CA	THR	A1047	-18.348	8.282	40.168	1.00	52.53	A
322	CB	THR	A1047	-18.350	6.810	40.436	1.00	53.10	A
323	OG1	THR	A1047	-19.609	6.362	40.991	1.00	49.98	A

324	CG2	THR	A1047	-17.193	6.440	41.295	1.00	55.96	A
325	C	THR	A1047	-19.668	9.016	40.509	1.00	54.13	A
326	O	THR	A1047	-19.798	9.737	41.505	1.00	51.28	A
327	N	LEU	A1048	-20.649	8.875	39.610	1.00	56.84	A
328	CA	LEU	A1048	-21.944	9.560	39.842	1.00	60.48	A
329	CB	LEU	A1048	-22.315	10.273	38.570	1.00	60.57	A
330	CG	LEU	A1048	-23.408	11.311	38.377	1.00	61.49	A
331	CD1	LEU	A1048	-22.720	12.338	37.463	1.00	56.88	A
332	CD2	LEU	A1048	-24.828	10.744	37.822	1.00	56.83	A
333	C	LEU	A1048	-22.988	8.554	40.373	1.00	61.68	A
334	O	LEU	A1048	-22.738	7.328	40.315	1.00	63.95	A
335	N	GLU	A1049	-24.093	9.030	40.942	1.00	63.28	A
336	CA	GLU	A1049	-24.963	8.193	41.909	1.00	65.68	A
337	CB	GLU	A1049	-25.196	9.064	43.135	1.00	63.34	A
338	CG	GLU	A1049	-25.022	8.332	44.443	1.00	64.20	A
339	CD	GLU	A1049	-23.793	7.344	44.495	1.00	67.57	A
340	OE1	GLU	A1049	-23.579	6.460	45.426	1.00	56.24	A
341	OE2	GLU	A1049	-23.030	7.472	43.530	1.00	72.03	A
342	C	GLU	A1049	-26.325	7.311	41.509	1.00	67.14	A
343	O	GLU	A1049	-27.069	7.559	40.511	1.00	67.34	A
344	N	ASN	A1050	-26.592	6.273	42.319	1.00	68.93	A
345	CA	ASN	A1050	-27.764	5.349	42.315	1.00	69.51	A
346	CB	ASN	A1050	-27.545	4.196	43.290	1.00	69.29	A
347	CG	ASN	A1050	-26.906	2.987	42.665	1.00	75.36	A
348	OD1	ASN	A1050	-25.679	2.820	42.744	1.00	78.45	A
349	ND2	ASN	A1050	-27.737	2.063	42.120	1.00	80.85	A
350	C	ASN	A1050	-29.084	5.937	42.842	1.00	71.36	A
351	O	ASN	A1050	-29.122	6.371	44.029	1.00	71.37	A
352	N	PRO	A1051	-30.191	5.738	42.037	1.00	71.73	A
353	CD	PRO	A1051	-30.298	4.529	41.192	1.00	71.02	A
354	CA	PRO	A1051	-31.405	6.475	41.929	1.00	71.56	A
355	CB	PRO	A1051	-32.435	5.363	42.077	1.00	73.05	A
356	CG	PRO	A1051	-31.563	3.946	41.674	1.00	71.00	A
357	C	PRO	A1051	-31.475	7.460	43.084	1.00	72.99	A
358	O	PRO	A1051	-31.784	7.039	44.230	1.00	73.02	A
359	N	PRO	A1052	-30.922	8.712	42.888	1.00	72.66	A
360	CD	PRO	A1052	-29.663	9.182	42.223	1.00	70.84	A
361	CA	PRO	A1052	-31.469	9.717	43.894	1.00	70.92	A
362	CB	PRO	A1052	-30.444	10.916	43.848	1.00	72.03	A
363	CG	PRO	A1052	-28.996	10.029	43.444	1.00	71.02	A
364	C	PRO	A1052	-32.960	9.936	43.809	1.00	68.27	A
365	O	PRO	A1052	-33.604	8.838	44.021	1.00	65.07	A
366	N	SER	A1057	-33.444	14.359	44.475	1.00	63.42	A
367	CA	SER	A1057	-34.318	14.468	43.314	1.00	64.32	A
368	CB	SER	A1057	-35.322	15.553	43.606	1.00	66.51	A
369	OG	SER	A1057	-34.585	16.798	43.673	1.00	70.24	A
370	C	SER	A1057	-33.653	14.753	41.924	1.00	64.44	A
371	O	SER	A1057	-33.476	13.817	41.215	1.00	67.06	A
372	N	ALA	A1058	-33.325	16.027	41.553	1.00	63.17	A
373	CA	ALA	A1058	-32.898	16.527	40.192	1.00	60.13	A
374	CB	ALA	A1058	-33.256	17.905	40.074	1.00	56.63	A
375	C	ALA	A1058	-31.425	16.428	40.102	1.00	59.93	A
376	O	ALA	A1058	-30.757	16.399	39.054	1.00	57.61	A
377	N	ALA	A1059	-30.907	16.309	41.315	1.00	61.50	A
378	CA	ALA	A1059	-29.494	16.502	41.612	1.00	59.67	A
379	CB	ALA	A1059	-29.431	17.377	42.760	1.00	61.08	A

380	C	ALA	A1059	-28.707	15.237	41.840	1.00	58.62	A
381	O	ALA	A1059	-29.257	14.070	41.943	1.00	61.34	A
382	N	VAL	A1060	-27.407	15.424	41.911	1.00	57.35	A
383	CA	VAL	A1060	-26.487	14.300	42.007	1.00	55.63	A
384	CB	VAL	A1060	-25.693	14.247	40.654	1.00	58.16	A
385	CG1	VAL	A1060	-26.718	14.045	39.336	1.00	53.15	A
386	CG2	VAL	A1060	-24.675	15.523	40.640	1.00	50.87	A
387	C	VAL	A1060	-25.368	14.499	43.032	1.00	55.20	A
388	O	VAL	A1060	-24.975	15.630	43.350	1.00	52.12	A
389	N	CYS	A1061	-24.800	13.346	43.423	1.00	55.62	A
390	CA	CYS	A1061	-23.539	13.251	44.177	1.00	55.25	A
391	CB	CYS	A1061	-23.823	12.788	45.656	1.00	55.10	A
392	SG	CYS	A1061	-25.650	12.699	46.018	1.00	57.66	A
393	C	CYS	A1061	-22.367	12.419	43.515	1.00	55.44	A
394	O	CYS	A1061	-22.547	11.540	42.679	1.00	58.20	A
395	N	LEU	A1062	-21.153	12.719	43.919	1.00	53.61	A
396	CA	LEU	A1062	-20.035	12.273	43.265	1.00	51.95	A
397	CB	LEU	A1062	-19.330	13.501	42.588	1.00	54.30	A
398	CG	LEU	A1062	-19.619	14.436	41.370	1.00	52.80	A
399	CD1	LEU	A1062	-21.022	14.893	41.275	1.00	50.19	A
400	CD2	LEU	A1062	-18.649	15.672	41.318	1.00	49.44	A
401	C	LEU	A1062	-19.125	11.785	44.420	1.00	51.88	A
402	O	LEU	A1062	-18.788	12.623	45.413	1.00	50.85	A
403	N	ARG	A1063	-18.658	10.529	44.250	1.00	46.31	A
404	CA	ARG	A1063	-17.838	10.002	45.186	1.00	45.80	A
405	CB	ARG	A1063	-18.500	8.949	46.044	1.00	49.53	A
406	CG	ARG	A1063	-19.272	7.714	45.395	1.00	52.99	A
407	CD	ARG	A1063	-18.686	6.485	46.142	1.00	53.69	A
408	NE	ARG	A1063	-19.659	5.621	46.660	1.00	52.00	A
409	CZ	ARG	A1063	-19.291	4.458	47.074	1.00	52.14	A
410	NH1	ARG	A1063	-18.017	4.283	47.085	1.00	46.67	A
411	NH2	ARG	A1063	-20.185	3.572	47.583	1.00	56.13	A
412	C	ARG	A1063	-16.555	9.646	44.611	1.00	44.08	A
413	O	ARG	A1063	-16.525	9.592	43.355	1.00	43.08	A
414	N	SER	A1064	-15.503	9.597	45.479	1.00	40.24	A
415	CA	SER	A1064	-14.189	9.347	45.082	1.00	41.91	A
416	CB	SER	A1064	-13.244	9.946	46.046	1.00	41.70	A
417	OG	SER	A1064	-13.882	10.026	47.256	1.00	51.98	A
418	C	SER	A1064	-13.969	7.881	45.087	1.00	43.92	A
419	O	SER	A1064	-14.863	7.149	45.494	1.00	43.09	A
420	N	HIS	A1065	-12.826	7.382	44.602	1.00	47.72	A
421	CA	HIS	A1065	-12.549	5.926	44.774	1.00	50.85	A
422	CB	HIS	A1065	-11.220	5.487	44.284	1.00	48.86	A
423	CG	HIS	A1065	-11.241	4.052	43.765	1.00	54.02	A
424	CD2	HIS	A1065	-10.256	3.298	43.207	1.00	59.11	A
425	ND1	HIS	A1065	-12.376	3.284	43.683	1.00	54.21	A
426	CE1	HIS	A1065	-12.045	2.082	43.246	1.00	63.10	A
427	NE2	HIS	A1065	-10.758	2.066	42.944	1.00	52.59	A
428	C	HIS	A1065	-12.518	5.383	46.197	1.00	55.25	A
429	O	HIS	A1065	-12.760	4.106	46.437	1.00	57.42	A
430	N	LEU	A1066	-12.115	6.286	47.139	1.00	55.58	A
431	CA	LEU	A1066	-11.741	5.859	48.466	1.00	52.27	A
432	CB	LEU	A1066	-11.022	6.953	49.171	1.00	52.78	A
433	CG	LEU	A1066	-9.495	7.143	48.817	1.00	53.96	A
434	CD1	LEU	A1066	-9.026	8.757	48.914	1.00	51.52	A
435	CD2	LEU	A1066	-8.504	6.115	49.444	1.00	40.36	A

436	C	LEU	A1066	-13.112	5.666	48.956	1.00	52.84	A
437	O	LEU	A1066	-13.353	4.828	49.917	1.00	55.58	A
438	N	GLY	A1067	-14.038	6.252	48.196	1.00	48.20	A
439	CA	GLY	A1067	-15.421	6.067	48.484	1.00	47.05	A
440	C	GLY	A1067	-16.057	7.204	49.282	1.00	47.29	A
441	O	GLY	A1067	-17.138	7.044	49.806	1.00	48.11	A
442	N	ARG	A1068	-15.479	8.405	49.360	1.00	47.32	A
443	CA	ARG	A1068	-16.168	9.406	50.205	1.00	49.64	A
444	CB	ARG	A1068	-15.094	10.122	50.989	1.00	49.69	A
445	CG	ARG	A1068	-14.137	9.211	51.539	1.00	42.24	A
446	CD	ARG	A1068	-14.887	8.456	52.478	1.00	41.23	A
447	NE	ARG	A1068	-13.990	7.748	53.372	1.00	51.66	A
448	CZ	ARG	A1068	-14.026	7.899	54.695	1.00	56.52	A
449	NH1	ARG	A1068	-15.020	8.603	55.411	1.00	49.15	A
450	NH2	ARG	A1068	-13.079	7.279	55.312	1.00	52.95	A
451	C	ARG	A1068	-16.736	10.307	49.135	1.00	51.50	A
452	O	ARG	A1068	-16.215	10.169	48.004	1.00	53.24	A
453	N	TYR	A1069	-17.692	11.194	49.436	1.00	47.45	A
454	CA	TYR	A1069	-18.345	11.885	48.405	1.00	47.50	A
455	CB	TYR	A1069	-19.789	11.932	48.778	1.00	51.64	A
456	CG	TYR	A1069	-20.442	10.525	48.640	1.00	57.11	A
457	CD1	TYR	A1069	-21.287	10.272	47.577	1.00	61.24	A
458	CE1	TYR	A1069	-21.858	9.071	47.417	1.00	65.65	A
459	CD2	TYR	A1069	-20.111	9.439	49.482	1.00	62.48	A
460	CE2	TYR	A1069	-20.652	8.187	49.291	1.00	60.12	A
461	CZ	TYR	A1069	-21.558	8.006	48.251	1.00	62.30	A
462	OH	TYR	A1069	-22.239	6.815	47.917	1.00	57.76	A
463	C	TYR	A1069	-17.727	13.245	48.152	1.00	48.56	A
464	O	TYR	A1069	-16.486	13.308	47.842	1.00	51.36	A
465	N	LEU	A1070	-18.462	14.362	48.284	1.00	43.32	A
466	CA	LEU	A1070	-17.870	15.704	48.089	1.00	42.37	A
467	CB	LEU	A1070	-18.070	16.149	46.581	1.00	43.29	A
468	CG	LEU	A1070	-17.221	17.196	45.814	1.00	41.01	A
469	CD1	LEU	A1070	-15.633	17.104	45.982	1.00	29.40	A
470	CD2	LEU	A1070	-17.603	17.432	44.361	1.00	36.72	A
471	C	LEU	A1070	-18.839	16.565	48.804	1.00	44.22	A
472	O	LEU	A1070	-20.013	16.504	48.428	1.00	46.64	A
473	N	ALA	A1071	-18.503	17.352	49.823	1.00	44.19	A
474	CA	ALA	A1071	-19.594	18.199	50.357	1.00	44.99	A
475	CB	ALA	A1071	-19.924	17.889	51.767	1.00	42.78	A
476	C	ALA	A1071	-19.234	19.643	50.190	1.00	46.02	A
477	O	ALA	A1071	-17.982	20.019	50.094	1.00	46.31	A
478	N	ALA	A1072	-20.254	20.455	50.242	1.00	46.45	A
479	CA	ALA	A1072	-19.987	21.889	50.285	1.00	50.39	A
480	CB	ALA	A1072	-20.185	22.467	48.958	1.00	50.40	A
481	C	ALA	A1072	-20.835	22.626	51.331	1.00	53.13	A
482	O	ALA	A1072	-22.076	22.752	51.181	1.00	55.34	A
483	N	ASP	A1073	-20.224	23.094	52.435	1.00	53.60	A
484	CA	ASP	A1073	-21.124	23.722	53.441	1.00	52.65	A
485	CB	ASP	A1073	-20.677	23.401	54.891	1.00	53.33	A
486	CG	ASP	A1073	-19.193	23.084	54.999	1.00	56.93	A
487	OD1	ASP	A1073	-18.533	23.310	56.080	1.00	61.74	A
488	OD2	ASP	A1073	-18.668	22.632	53.932	1.00	62.41	A
489	C	ASP	A1073	-21.368	25.224	53.162	1.00	52.27	A
490	O	ASP	A1073	-20.776	25.830	52.346	1.00	51.94	A
491	N	LYS	A1074	-22.289	25.845	53.857	1.00	54.57	A

492	CA	LYS	A1074	-22.733	27.147	53.526	1.00	53.80	A
493	CB	LYS	A1074	-23.996	27.448	54.360	1.00	56.45	A
494	CG	LYS	A1074	-25.470	27.116	53.659	1.00	58.21	A
495	CD	LYS	A1074	-26.664	27.495	54.668	1.00	54.48	A
496	CE	LYS	A1074	-28.006	27.670	53.988	1.00	49.89	A
497	NZ	LYS	A1074	-28.898	28.147	54.991	1.00	53.66	A
498	C	LYS	A1074	-21.587	28.107	53.702	1.00	53.97	A
499	O	LYS	A1074	-21.744	29.261	53.893	1.00	54.47	A
500	N	ASP	A1075	-20.380	27.632	53.542	1.00	55.26	A
501	CA	ASP	A1075	-19.256	28.540	53.600	1.00	53.97	A
502	CB	ASP	A1075	-18.538	28.249	54.943	1.00	54.71	A
503	CG	ASP	A1075	-19.426	28.620	56.078	1.00	55.41	A
504	OD1	ASP	A1075	-20.372	27.857	56.312	1.00	58.04	A
505	OD2	ASP	A1075	-19.275	29.774	56.571	1.00	54.16	A
506	C	ASP	A1075	-18.238	28.425	52.565	1.00	54.10	A
507	O	ASP	A1075	-17.161	29.039	52.837	1.00	55.78	A
508	N	GLY	A1076	-18.451	27.546	51.520	1.00	52.33	A
509	CA	GLY	A1076	-17.481	27.255	50.455	1.00	50.05	A
510	C	GLY	A1076	-16.520	26.162	50.876	1.00	51.21	A
511	O	GLY	A1076	-15.550	25.813	50.218	1.00	52.93	A
512	N	ASN	A1077	-16.641	25.642	52.049	1.00	48.90	A
513	CA	ASN	A1077	-15.745	24.516	52.235	1.00	49.47	A
514	CB	ASN	A1077	-15.991	24.020	53.651	1.00	50.95	A
515	CG	ASN	A1077	-16.396	25.019	54.441	1.00	46.43	A
516	OD1	ASN	A1077	-15.581	25.912	54.708	1.00	56.36	A
517	ND2	ASN	A1077	-17.648	25.046	54.749	1.00	48.43	A
518	C	ASN	A1077	-15.921	23.256	51.410	1.00	49.14	A
519	O	ASN	A1077	-17.005	22.569	51.480	1.00	50.93	A
520	N	VAL	A1078	-14.832	22.791	50.849	1.00	49.40	A
521	CA	VAL	A1078	-14.872	21.472	50.162	1.00	48.53	A
522	CB	VAL	A1078	-14.553	21.475	48.652	1.00	46.65	A
523	CG1	VAL	A1078	-13.935	22.562	48.333	1.00	30.89	A
524	CG2	VAL	A1078	-13.771	20.086	48.225	1.00	45.09	A
525	C	VAL	A1078	-14.285	20.270	50.836	1.00	51.34	A
526	O	VAL	A1078	-13.058	20.147	51.063	1.00	54.53	A
527	N	THR	A1079	-15.203	19.379	51.179	1.00	51.30	A
528	CA	THR	A1079	-14.791	18.183	51.855	1.00	49.51	A
529	CB	THR	A1079	-15.281	18.180	53.248	1.00	48.77	A
530	OG1	THR	A1079	-16.519	18.910	53.302	1.00	48.75	A
531	CG2	THR	A1079	-14.232	18.816	54.155	1.00	43.68	A
532	C	THR	A1079	-15.313	17.001	51.032	1.00	51.17	A
533	O	THR	A1079	-16.382	17.061	50.444	1.00	52.70	A
534	N	CYS	A1080	-14.398	16.068	50.841	1.00	49.63	A
535	CA	CYS	A1080	-14.615	14.818	50.382	1.00	49.93	A
536	CB	CYS	A1080	-13.731	14.719	49.248	1.00	45.32	A
537	SG	CYS	A1080	-14.144	13.142	48.423	1.00	45.31	A
538	C	CYS	A1080	-14.236	13.686	51.436	1.00	51.02	A
539	O	CYS	A1080	-13.245	13.033	51.292	1.00	52.54	A
540	N	GLU	A1081	-14.968	13.521	52.504	1.00	51.75	A
541	CA	GLU	A1081	-14.573	12.634	53.641	1.00	54.09	A
542	CB	GLU	A1081	-13.912	13.418	54.814	1.00	54.32	A
543	CG	GLU	A1081	-14.881	14.205	55.784	1.00	54.39	A
544	CD	GLU	A1081	-14.190	15.533	56.249	1.00	57.02	A
545	OE1	GLU	A1081	-14.909	16.473	56.764	1.00	54.50	A
546	OE2	GLU	A1081	-12.941	15.675	55.988	1.00	55.50	A
547	C	GLU	A1081	-15.774	11.825	54.256	1.00	55.38	A

548	O	GLU	A1081	-15.530	10.661	54.767	1.00	54.03	A
549	N	ARG	A1082	-17.010	12.437	54.201	1.00	55.32	A
550	CA	ARG	A1082	-18.255	11.729	54.441	1.00	57.01	A
551	CB	ARG	A1082	-19.383	12.668	54.716	1.00	59.69	A
552	CG	ARG	A1082	-19.836	13.586	53.585	1.00	64.08	A
553	CD	ARG	A1082	-20.463	14.900	54.257	1.00	65.95	A
554	NE	ARG	A1082	-21.770	14.552	54.770	1.00	72.82	A
555	CZ	ARG	A1082	-22.936	15.229	54.610	1.00	72.48	A
556	NH1	ARG	A1082	-23.014	16.412	53.925	1.00	57.84	A
557	NH2	ARG	A1082	-24.059	14.666	55.174	1.00	71.91	A
558	C	ARG	A1082	-18.723	10.668	53.476	1.00	57.07	A
559	O	ARG	A1082	-18.826	10.866	52.258	1.00	56.91	A
560	N	GLU	A1083	-18.973	9.509	54.096	1.00	56.68	A
561	CA	GLU	A1083	-19.322	8.214	53.428	1.00	56.23	A
562	CB	GLU	A1083	-18.834	7.097	54.238	1.00	52.11	A
563	CG	GLU	A1083	-19.304	7.301	55.604	1.00	56.40	A
564	CD	GLU	A1083	-18.842	6.215	56.509	1.00	65.36	A
565	OE1	GLU	A1083	-17.525	6.169	56.607	1.00	57.98	A
566	OE2	GLU	A1083	-19.784	5.386	57.003	1.00	62.74	A
567	C	GLU	A1083	-20.833	8.013	53.236	1.00	57.67	A
568	O	GLU	A1083	-21.228	7.201	52.398	1.00	57.89	A
569	N	VAL	A1084	-21.647	8.822	53.938	1.00	57.79	A
570	CA	VAL	A1084	-23.007	8.924	53.625	1.00	58.47	A
571	CB	VAL	A1084	-23.808	8.255	54.742	1.00	60.91	A
572	CG1	VAL	A1084	-25.381	8.538	54.673	1.00	59.38	A
573	CG2	VAL	A1084	-23.603	6.695	54.729	1.00	60.24	A
574	C	VAL	A1084	-23.406	10.401	53.399	1.00	59.76	A
575	O	VAL	A1084	-23.515	11.177	54.316	1.00	61.89	A
576	N	PRO	A1085	-23.538	10.797	52.163	1.00	59.08	A
577	CD	PRO	A1085	-22.730	10.194	51.109	1.00	61.69	A
578	CA	PRO	A1085	-24.347	11.754	51.516	1.00	59.94	A
579	CB	PRO	A1085	-24.994	10.855	50.402	1.00	58.86	A
580	CG	PRO	A1085	-23.825	10.041	49.937	1.00	58.73	A
581	C	PRO	A1085	-25.456	12.503	52.260	1.00	59.13	A
582	O	PRO	A1085	-26.461	11.867	52.450	1.00	59.92	A
583	N	GLY	A1086	-25.288	13.816	52.564	1.00	56.69	A
584	CA	GLY	A1086	-26.169	14.642	53.479	1.00	55.27	A
585	C	GLY	A1086	-26.800	15.722	52.627	1.00	53.00	A
586	O	GLY	A1086	-26.767	15.511	51.472	1.00	55.42	A
587	N	PRO	A1087	-27.472	16.779	53.125	1.00	52.87	A
588	CD	PRO	A1087	-28.323	16.922	54.328	1.00	55.67	A
589	CA	PRO	A1087	-27.774	17.905	52.192	1.00	53.56	A
590	CB	PRO	A1087	-28.574	18.893	53.004	1.00	50.99	A
591	CG	PRO	A1087	-29.386	17.981	53.814	1.00	55.52	A
592	C	PRO	A1087	-26.612	18.566	51.625	1.00	55.63	A
593	O	PRO	A1087	-26.749	19.384	50.621	1.00	58.05	A
594	N	ASP	A1088	-25.447	18.219	52.158	1.00	56.01	A
595	CA	ASP	A1088	-24.351	18.953	51.701	1.00	55.34	A
596	CB	ASP	A1088	-23.579	19.524	52.870	1.00	58.96	A
597	CG	ASP	A1088	-23.940	20.939	53.069	1.00	62.44	A
598	OD1	ASP	A1088	-24.435	21.394	54.131	1.00	67.96	A
599	OD2	ASP	A1088	-23.904	21.576	52.011	1.00	69.27	A
600	C	ASP	A1088	-23.594	18.346	50.594	1.00	54.12	A
601	O	ASP	A1088	-22.874	19.068	49.882	1.00	56.36	A
602	N	CYS	A1089	-23.825	17.097	50.300	1.00	50.47	A
603	CA	CYS	A1089	-23.078	16.490	49.218	1.00	50.41	A

604	CB	CYS	A1089	-22.851	15.027	49.651	1.00	49.53	A
605	SG	CYS	A1089	-21.907	14.459	51.307	1.00	54.68	A
606	C	CYS	A1089	-23.821	16.606	47.722	1.00	52.20	A
607	O	CYS	A1089	-23.338	15.997	46.746	1.00	51.41	A
608	N	ARG	A1090	-24.959	17.346	47.560	1.00	50.29	A
609	CA	ARG	A1090	-25.771	17.377	46.269	1.00	51.09	A
610	CB	ARG	A1090	-27.367	17.383	46.442	1.00	52.39	A
611	CG	ARG	A1090	-28.217	16.731	47.699	1.00	52.01	A
612	CD	ARG	A1090	-28.857	15.473	47.127	1.00	58.91	A
613	NE	ARG	A1090	-30.299	15.291	47.184	1.00	58.93	A
614	CZ	ARG	A1090	-31.230	16.250	47.029	1.00	66.98	A
615	NH1	ARG	A1090	-30.940	17.558	46.811	1.00	64.17	A
616	NH2	ARG	A1090	-32.515	15.907	47.139	1.00	67.07	A
617	C	ARG	A1090	-25.561	18.585	45.321	1.00	49.48	A
618	O	ARG	A1090	-26.102	19.672	45.545	1.00	46.66	A
619	N	PHE	A1091	-24.901	18.326	44.207	1.00	49.55	A
620	CA	PHE	A1091	-24.622	19.340	43.121	1.00	46.71	A
621	CB	PHE	A1091	-23.231	19.295	42.784	1.00	48.06	A
622	CG	PHE	A1091	-22.352	19.351	43.983	1.00	52.98	A
623	CD1	PHE	A1091	-21.779	20.553	44.378	1.00	54.19	A
624	CD2	PHE	A1091	-22.135	18.228	44.717	1.00	54.06	A
625	CE1	PHE	A1091	-20.968	20.640	45.519	1.00	56.13	A
626	CE2	PHE	A1091	-21.380	18.280	45.847	1.00	60.51	A
627	CZ	PHE	A1091	-20.744	19.494	46.248	1.00	60.12	A
628	C	PHE	A1091	-25.443	19.202	41.868	1.00	43.36	A
629	O	PHE	A1091	-26.309	18.445	41.768	1.00	42.69	A
630	N	LEU	A1092	-25.256	20.034	40.928	1.00	43.49	A
631	CA	LEU	A1092	-26.171	20.040	39.772	1.00	43.00	A
632	CB	LEU	A1092	-27.108	21.166	39.845	1.00	41.09	A
633	CG	LEU	A1092	-28.306	21.058	40.731	1.00	39.34	A
634	CD1	LEU	A1092	-28.414	22.398	41.184	1.00	38.60	A
635	CD2	LEU	A1092	-29.595	20.886	40.162	1.00	25.44	A
636	C	LEU	A1092	-25.201	20.389	38.766	1.00	42.42	A
637	O	LEU	A1092	-24.648	21.378	38.968	1.00	39.92	A
638	N	ILE	A1093	-24.872	19.462	37.842	1.00	45.45	A
639	CA	ILE	A1093	-24.237	19.706	36.518	1.00	46.07	A
640	CB	ILE	A1093	-24.448	18.594	35.561	1.00	44.66	A
641	CG2	ILE	A1093	-23.545	18.812	34.302	1.00	43.88	A
642	CG1	ILE	A1093	-24.033	17.206	36.167	1.00	44.44	A
643	CD1	ILE	A1093	-23.461	17.228	37.476	1.00	46.13	A
644	C	ILE	A1093	-24.903	20.853	35.885	1.00	48.03	A
645	O	ILE	A1093	-26.155	20.922	35.966	1.00	50.68	A
646	N	VAL	A1094	-24.116	21.818	35.391	1.00	49.43	A
647	CA	VAL	A1094	-24.768	22.791	34.466	1.00	55.65	A
648	CB	VAL	A1094	-25.009	24.187	35.170	1.00	56.33	A
649	CG1	VAL	A1094	-26.351	24.747	34.712	1.00	57.71	A
650	CG2	VAL	A1094	-25.137	23.974	36.779	1.00	55.27	A
651	C	VAL	A1094	-24.158	22.834	32.993	1.00	56.94	A
652	O	VAL	A1094	-23.191	23.546	32.749	1.00	60.96	A
653	N	ALA	A1095	-24.592	22.015	32.030	1.00	55.92	A
654	CA	ALA	A1095	-23.968	22.172	30.683	1.00	56.02	A
655	CB	ALA	A1095	-24.415	21.097	29.689	1.00	55.70	A
656	C	ALA	A1095	-24.075	23.515	30.021	1.00	55.99	A
657	O	ALA	A1095	-25.174	24.238	29.973	1.00	56.99	A
658	N	HIS	A1096	-22.947	23.818	29.417	1.00	57.87	A
659	CA	HIS	A1096	-22.677	25.191	28.954	1.00	61.82	A

660	CB	HIS	A1096	-21.590	25.857	29.751	1.00	60.24	A
661	CG	HIS	A1096	-22.112	26.381	31.032	1.00	59.56	A
662	CD2	HIS	A1096	-21.537	26.509	32.246	1.00	64.07	A
663	ND1	HIS	A1096	-23.420	26.803	31.164	1.00	52.40	A
664	CE1	HIS	A1096	-23.617	27.199	32.399	1.00	64.14	A
665	NE2	HIS	A1096	-22.491	27.021	33.087	1.00	67.16	A
666	C	HIS	A1096	-22.411	25.271	27.475	1.00	64.40	A
667	O	HIS	A1096	-21.172	25.236	27.020	1.00	64.38	A
668	N	ASP	A1097	-23.595	25.237	26.741	1.00	65.38	A
669	CA	ASP	A1097	-23.670	25.448	25.350	1.00	66.57	A
670	CB	ASP	A1097	-24.030	26.906	24.999	1.00	66.95	A
671	CG	ASP	A1097	-25.524	27.280	25.285	1.00	71.79	A
672	OD1	ASP	A1097	-25.884	28.224	24.572	1.00	73.85	A
673	OD2	ASP	A1097	-26.311	26.699	26.115	1.00	71.77	A
674	C	ASP	A1097	-22.246	25.282	25.111	1.00	65.98	A
675	O	ASP	A1097	-21.658	24.264	25.456	1.00	69.86	A
676	N	ASP	A1098	-21.594	26.308	24.693	1.00	65.57	A
677	CA	ASP	A1098	-20.237	26.117	24.352	1.00	65.74	A
678	CB	ASP	A1098	-20.114	26.985	23.143	1.00	67.00	A
679	CG	ASP	A1098	-21.226	26.733	22.063	1.00	73.26	A
680	OD1	ASP	A1098	-22.380	26.278	22.307	1.00	73.41	A
681	OD2	ASP	A1098	-20.842	27.090	20.882	1.00	78.59	A
682	C	ASP	A1098	-18.993	26.354	25.415	1.00	65.81	A
683	O	ASP	A1098	-18.006	27.082	25.239	1.00	65.17	A
684	N	GLY	A1099	-18.793	25.501	26.471	1.00	64.28	A
685	CA	GLY	A1099	-17.621	25.875	27.314	1.00	63.47	A
686	C	GLY	A1099	-17.509	24.473	27.857	1.00	63.88	A
687	O	GLY	A1099	-17.146	23.490	27.059	1.00	63.26	A
688	N	ARG	A1100	-17.991	24.317	29.109	1.00	61.08	A
689	CA	ARG	A1100	-17.789	23.096	29.897	1.00	57.01	A
690	CB	ARG	A1100	-16.519	23.407	30.720	1.00	58.35	A
691	CG	ARG	A1100	-15.173	23.592	29.838	1.00	53.42	A
692	CD	ARG	A1100	-14.106	24.004	30.799	1.00	52.12	A
693	NE	ARG	A1100	-14.623	25.343	30.934	1.00	52.10	A
694	CZ	ARG	A1100	-13.882	26.433	31.028	1.00	46.76	A
695	NH1	ARG	A1100	-12.560	26.304	31.190	1.00	42.27	A
696	NH2	ARG	A1100	-14.529	27.596	31.061	1.00	36.94	A
697	C	ARG	A1100	-19.031	22.782	30.752	1.00	55.62	A
698	O	ARG	A1100	-20.107	22.924	30.231	1.00	52.91	A
699	N	TRP	A1101	-18.887	22.309	32.004	1.00	54.88	A
700	CA	TRP	A1101	-20.029	22.095	32.989	1.00	57.27	A
701	CB	TRP	A1101	-19.758	20.760	33.656	1.00	58.05	A
702	CG	TRP	A1101	-20.439	19.614	32.937	1.00	64.92	A
703	CD2	TRP	A1101	-20.578	18.224	33.403	1.00	69.91	A
704	CE2	TRP	A1101	-21.382	17.542	32.458	1.00	69.98	A
705	CE3	TRP	A1101	-20.144	17.521	34.537	1.00	68.13	A
706	CD1	TRP	A1101	-21.085	19.673	31.724	1.00	65.96	A
707	NE1	TRP	A1101	-21.685	18.438	31.451	1.00	69.40	A
708	CZ2	TRP	A1101	-21.742	16.211	32.625	1.00	62.24	A
709	CZ3	TRP	A1101	-20.508	16.184	34.689	1.00	62.33	A
710	CH2	TRP	A1101	-21.297	15.558	33.753	1.00	62.00	A
711	C	TRP	A1101	-20.284	23.258	34.108	1.00	55.94	A
712	O	TRP	A1101	-19.585	24.293	34.043	1.00	53.62	A
713	N	SER	A1102	-21.262	23.132	35.057	1.00	55.99	A
714	CA	SER	A1102	-21.056	23.830	36.411	1.00	58.45	A
715	CB	SER	A1102	-21.300	25.392	36.386	1.00	58.51	A

716	OG	SER A1102	-20.179	26.219	35.938	1.00	54.55	A
717	C	SER A1102	-21.641	23.306	37.756	1.00	59.31	A
718	O	SER A1102	-22.782	23.673	38.140	1.00	59.33	A
719	N	LEU A1103	-20.811	22.573	38.501	1.00	59.63	A
720	CA	LEU A1103	-21.107	22.083	39.892	1.00	60.50	A
721	CB	LEU A1103	-19.933	21.276	40.443	1.00	59.64	A
722	CG	LEU A1103	-19.879	19.787	40.183	1.00	59.22	A
723	CD1	LEU A1103	-21.124	19.102	40.780	1.00	52.84	A
724	CD2	LEU A1103	-19.715	19.555	38.588	1.00	59.39	A
725	C	LEU A1103	-21.493	23.167	40.937	1.00	61.43	A
726	O	LEU A1103	-20.610	23.691	41.723	1.00	62.71	A
727	N	GLN A1104	-22.784	23.532	40.876	1.00	60.17	A
728	CA	GLN A1104	-23.431	24.334	41.845	1.00	60.57	A
729	CB	GLN A1104	-24.451	25.083	41.105	1.00	58.35	A
730	CG	GLN A1104	-25.497	25.686	42.051	1.00	60.90	A
731	CD	GLN A1104	-26.876	25.893	41.317	1.00	56.31	A
732	OE1	GLN A1104	-26.976	25.702	40.037	1.00	60.62	A
733	NE2	GLN A1104	-27.937	26.157	42.098	1.00	36.93	A
734	C	GLN A1104	-24.103	23.480	42.996	1.00	61.59	A
735	O	GLN A1104	-24.889	22.534	42.712	1.00	63.63	A
736	N	SER A1105	-23.868	23.840	44.268	1.00	60.16	A
737	CA	SER A1105	-24.666	23.339	45.405	1.00	56.98	A
738	CB	SER A1105	-23.931	23.612	46.729	1.00	57.37	A
739	OG	SER A1105	-24.702	23.243	47.875	1.00	61.71	A
740	C	SER A1105	-26.028	23.983	45.391	1.00	56.48	A
741	O	SER A1105	-26.273	25.192	45.088	1.00	58.43	A
742	N	GLU A1106	-26.979	23.170	45.716	1.00	55.66	A
743	CA	GLU A1106	-28.374	23.476	45.409	1.00	52.93	A
744	CB	GLU A1106	-28.988	22.165	45.019	1.00	52.65	A
745	CG	GLU A1106	-30.368	22.165	45.360	1.00	49.18	A
746	CD	GLU A1106	-30.895	20.778	45.549	1.00	49.36	A
747	OE1	GLU A1106	-30.180	19.914	46.140	1.00	45.18	A
748	OE2	GLU A1106	-32.056	20.570	45.097	1.00	50.68	A
749	C	GLU A1106	-29.119	23.889	46.638	1.00	53.58	A
750	O	GLU A1106	-30.186	24.534	46.521	1.00	49.78	A
751	N	ALA A1107	-28.586	23.402	47.799	1.00	52.93	A
752	CA	ALA A1107	-29.040	23.797	49.068	1.00	54.59	A
753	CB	ALA A1107	-28.115	23.238	50.151	1.00	54.41	A
754	C	ALA A1107	-29.033	25.353	48.970	1.00	56.73	A
755	O	ALA A1107	-30.090	25.933	48.908	1.00	56.16	A
756	N	HIS A1108	-27.846	25.990	48.797	1.00	57.42	A
757	CA	HIS A1108	-27.738	27.460	48.583	1.00	57.86	A
758	CB	HIS A1108	-26.552	27.953	49.472	1.00	56.49	A
759	CG	HIS A1108	-25.669	26.827	49.998	1.00	57.35	A
760	CD2	HIS A1108	-24.339	26.586	49.845	1.00	54.64	A
761	ND1	HIS A1108	-26.131	25.807	50.821	1.00	60.35	A
762	CE1	HIS A1108	-25.140	24.961	51.103	1.00	56.57	A
763	NE2	HIS A1108	-24.049	25.392	50.490	1.00	54.02	A
764	C	HIS A1108	-27.758	28.058	46.986	1.00	59.34	A
765	O	HIS A1108	-28.763	28.681	46.520	1.00	57.24	A
766	N	ARG A1109	-26.698	27.907	46.179	1.00	58.79	A
767	CA	ARG A1109	-26.754	28.555	44.894	1.00	59.92	A
768	CB	ARG A1109	-27.415	29.876	44.981	1.00	59.48	A
769	CG	RG A1109	-28.212	30.291	43.693	1.00	65.60	A
770	CD	ARG A1109	-29.793	30.040	43.872	1.00	65.13	A
771	NE	ARG A1109	-30.015	28.757	44.614	1.00	65.11	A

772	CZ	ARG A1109	-31.172	28.349	45.173	1.00	61.19	A
773	NH1	ARG A1109	-32.316	29.022	45.071	1.00	66.22	A
774	NH2	ARG A1109	-31.212	27.243	45.803	1.00	50.65	A
775	C	ARG A1109	-25.337	28.777	44.425	1.00	62.56	A
776	O	ARG A1109	-25.059	29.348	43.326	1.00	61.66	A
777	N	ARG A1110	-24.436	28.251	45.244	1.00	62.88	A
778	CA	ARG A1110	-23.128	28.796	45.267	1.00	63.89	A
779	CB	ARG A1110	-22.878	29.111	46.765	1.00	65.61	A
780	CG	ARG A1110	-24.131	29.891	47.521	1.00	67.17	A
781	CD	ARG A1110	-23.942	31.372	48.192	1.00	61.85	A
782	NE	ARG A1110	-22.648	32.008	47.860	1.00	60.65	A
783	CZ	ARG A1110	-22.375	33.323	48.025	1.00	60.78	A
784	NH1	ARG A1110	-23.336	34.143	48.475	1.00	56.21	A
785	NH2	ARG A1110	-21.176	33.838	47.671	1.00	55.22	A
786	C	ARG A1110	-22.137	27.752	44.627	1.00	64.51	A
787	O	ARG A1110	-22.293	26.533	44.796	1.00	66.52	A
788	N	TYR A1111	-21.137	28.186	43.852	1.00	64.43	A
789	CA	TYR A1111	-20.620	27.344	42.642	1.00	61.77	A
790	CB	TYR A1111	-20.693	28.092	41.305	1.00	60.54	A
791	CG	TYR A1111	-22.067	28.239	40.669	1.00	60.49	A
792	CD1	TYR A1111	-22.894	29.331	40.900	1.00	60.72	A
793	CE1	TYR A1111	-24.231	29.379	40.202	1.00	65.30	A
794	CD2	TYR A1111	-22.509	27.295	39.752	1.00	59.93	A
795	CE2	TYR A1111	-23.755	27.306	39.123	1.00	56.46	A
796	CZ	TYR A1111	-24.610	28.312	39.320	1.00	64.19	A
797	OH	TYR A1111	-25.809	28.214	38.620	1.00	64.45	A
798	C	TYR A1111	-19.234	26.824	42.878	1.00	59.21	A
799	O	TYR A1111	-18.492	27.456	43.620	1.00	58.87	A
800	N	PHE A1112	-18.926	25.677	42.286	1.00	55.53	A
801	CA	PHE A1112	-17.680	25.041	42.547	1.00	53.95	A
802	CB	PHE A1112	-17.838	23.505	42.331	1.00	55.37	A
803	CG	PHE A1112	-16.650	22.647	42.851	1.00	57.19	A
804	CD1	PHE A1112	-16.402	22.495	44.256	1.00	55.82	A
805	CD2	PHE A1112	-15.834	21.944	41.957	1.00	53.96	A
806	CE1	PHE A1112	-15.338	21.654	44.750	1.00	55.78	A
807	CE2	PHE A1112	-14.789	21.075	42.442	1.00	59.75	A
808	CZ	PHE A1112	-14.543	20.925	43.877	1.00	56.33	A
809	C	PHE A1112	-16.721	25.619	41.624	1.00	51.64	A
810	O	PHE A1112	-17.122	25.849	40.522	1.00	53.63	A
811	N	LY A1113	-15.452	25.792	42.021	1.00	50.07	A
812	CA	GLY A1113	-14.379	26.364	41.198	1.00	46.39	A
813	C	GLY A1113	-13.057	26.434	41.989	1.00	47.92	A
814	O	GLY A1113	-12.917	25.822	43.019	1.00	48.18	A
815	N	GLY A1114	-12.011	27.132	41.494	1.00	50.72	A
816	CA	GLY A1114	-10.633	27.180	42.183	1.00	49.80	A
817	C	GLY A1114	-9.479	26.725	41.368	1.00	52.50	A
818	O	GLY A1114	-9.551	26.561	40.089	1.00	55.00	A
819	N	THR A1115	-8.355	26.526	42.037	1.00	52.05	A
820	CA	THR A1115	-7.364	25.556	41.509	1.00	50.12	A
821	CB	THR A1115	-6.587	25.946	40.303	1.00	51.01	A
822	OG1	THR A1115	-5.528	24.902	40.101	1.00	56.05	A
823	CG2	THR A1115	-6.011	27.492	40.407	1.00	47.32	A
824	C	THR A1115	-6.447	25.173	42.608	1.00	50.16	A
825	O	THR A1115	-6.826	25.252	43.730	1.00	51.80	A
826	N	GLU A1116	-5.301	24.636	42.293	1.00	49.91	A
827	CA	GLU A1116	-4.563	23.746	43.174	1.00	51.63	A

828	CB	GLU	A1116	-3.179	24.458	43.488	1.00	54.50	A
829	CG	GLU	A1116	-1.860	23.673	43.060	1.00	59.58	A
830	CD	GLU	A1116	-1.660	23.532	41.469	1.00	69.91	A
831	OE1	GLU	A1116	-1.168	22.430	41.020	1.00	62.25	A
832	OE2	GLU	A1116	-2.076	24.504	40.683	1.00	73.04	A
833	C	GLU	A1116	-5.338	23.019	44.402	1.00	50.87	A
834	O	GLU	A1116	-6.482	22.600	44.325	1.00	50.01	A
835	N	ASP	A1117	-4.677	22.828	45.515	1.00	51.93	A
836	CA	ASP	A1117	-5.336	22.355	46.719	1.00	53.11	A
837	CB	ASP	A1117	-4.255	21.965	47.750	1.00	52.31	A
838	CG	ASP	A1117	-3.636	23.209	48.392	1.00	61.16	A
839	OD1	ASP	A1117	-4.419	24.243	48.358	1.00	72.16	A
840	OD2	ASP	A1117	-2.489	23.194	48.958	1.00	58.91	A
841	C	ASP	A1117	-6.108	23.568	47.178	1.00	51.47	A
842	O	ASP	A1117	-6.344	23.769	48.348	1.00	49.95	A
843	N	ARG	A1118	-6.420	24.420	46.254	1.00	51.96	A
844	CA	ARG	A1118	-7.143	25.627	46.653	1.00	54.21	A
845	CB	ARG	A1118	-6.306	26.857	46.406	1.00	53.19	A
846	CG	ARG	A1118	-6.983	28.233	46.695	1.00	56.03	A
847	CD	ARG	A1118	-6.768	28.869	48.164	1.00	51.44	A
848	NE	ARG	A1118	-7.847	28.342	48.939	1.00	54.38	A
849	CZ	ARG	A1118	-7.987	28.424	50.258	1.00	54.87	A
850	NH1	ARG	A1118	-7.078	29.079	50.892	1.00	49.46	A
851	NH2	ARG	A1118	-9.081	27.880	50.902	1.00	58.50	A
852	C	ARG	A1118	-8.565	25.766	45.997	1.00	54.93	A
853	O	ARG	A1118	-8.935	26.812	45.436	1.00	56.90	A
854	N	LEU	A1119	-9.328	24.689	46.059	1.00	52.65	A
855	CA	LEU	A1119	-10.565	24.634	45.469	1.00	51.53	A
856	CB	LEU	A1119	-10.727	23.173	45.089	1.00	50.26	A
857	CG	LEU	A1119	-11.264	23.096	43.669	1.00	53.50	A
858	CD1	LEU	A1119	-10.517	23.536	42.356	1.00	49.79	A
859	CD2	LEU	A1119	-11.660	21.723	43.575	1.00	58.40	A
860	C	LEU	A1119	-11.467	24.996	46.605	1.00	53.21	A
861	O	LEU	A1119	-11.105	24.794	47.828	1.00	56.04	A
862	N	SER	A1120	-12.683	25.399	46.235	1.00	52.68	A
863	CA	SER	A1120	-13.752	25.757	47.109	1.00	51.28	A
864	CB	SER	A1120	-13.504	27.116	47.796	1.00	53.56	A
865	OG	SER	A1120	-14.080	28.270	47.105	1.00	56.69	A
866	C	SER	A1120	-14.879	25.981	46.205	1.00	52.16	A
867	O	SER	A1120	-14.770	25.877	44.976	1.00	55.08	A
868	N	CYS	A1121	-15.909	26.524	46.790	1.00	51.98	A
869	CA	CYS	A1121	-17.169	26.590	46.205	1.00	53.07	A
870	CB	CYS	A1121	-17.821	25.112	46.167	1.00	50.71	A
871	SG	CYS	A1121	-19.698	24.993	45.537	1.00	56.99	A
872	C	CYS	A1121	-17.966	27.702	46.987	1.00	51.67	A
873	O	CYS	A1121	-19.205	27.676	47.019	1.00	52.16	A
874	N	PHE	A1122	-17.289	28.706	47.532	1.00	54.09	A
875	CA	PHE	A1122	-18.021	29.935	48.182	1.00	56.20	A
876	CB	PHE	A1122	-17.084	30.892	48.975	1.00	57.40	A
877	CG	PHE	A1122	-17.765	32.155	49.496	1.00	56.22	A
878	CD1	PHE	A1122	-17.649	33.383	48.813	1.00	58.42	A
879	CD2	PHE	A1122	-18.541	32.105	50.646	1.00	55.60	A
880	CE1	PHE	A1122	-18.322	34.551	49.317	1.00	57.88	A
881	CE2	PHE	A1122	-19.245	33.206	51.129	1.00	53.13	A
882	CZ	PHE	A1122	-19.154	34.440	50.444	1.00	58.16	A
883	C	PHE	A1122	-18.796	30.802	47.177	1.00	58.70	A

884	O	PHE	A1122	-19.692	31.631	47.562	1.00	58.90	A
885	N	ALA	A1123	-18.479	30.512	45.888	1.00	58.30	A
886	CA	ALA	A1123	-18.293	31.487	44.886	1.00	57.01	A
887	CB	ALA	A1123	-17.247	31.030	44.005	1.00	53.13	A
888	C	ALA	A1123	-19.609	31.418	44.210	1.00	59.39	A
889	O	ALA	A1123	-19.689	30.622	43.350	1.00	62.92	A
890	N	GLN	A1124	-20.592	32.248	44.565	1.00	58.59	A
891	CA	GLN	A1124	-21.892	32.263	44.036	1.00	60.33	A
892	CB	GLN	A1124	-22.797	33.004	45.023	1.00	61.66	A
893	CG	GLN	A1124	-22.699	34.627	45.106	1.00	60.20	A
894	CD	GLN	A1124	-24.007	35.186	45.928	1.00	65.71	A
895	OE1	GLN	A1124	-24.051	36.374	46.385	1.00	74.45	A
896	NE2	GLN	A1124	-25.051	34.322	46.103	1.00	56.96	A
897	C	GLN	A1124	-22.177	32.781	42.568	1.00	60.29	A
898	O	GLN	A1124	-23.411	33.090	42.248	1.00	57.22	A
899	N	THR	A1125	-21.127	32.779	41.696	1.00	59.56	A
900	CA	THR	A1125	-21.244	33.108	40.199	1.00	60.01	A
901	CB	THR	A1125	-21.101	34.645	39.943	1.00	60.67	A
902	OG1	THR	A1125	-21.962	35.075	38.893	1.00	60.32	A
903	CG2	THR	A1125	-19.612	34.942	39.517	1.00	57.52	A
904	C	THR	A1125	-20.113	32.420	39.260	1.00	61.10	A
905	O	THR	A1125	-19.204	31.750	39.763	1.00	62.25	A
906	N	VAL	A1126	-20.114	32.595	37.914	1.00	59.92	A
907	CA	VAL	A1126	-19.246	31.780	37.099	1.00	57.37	A
908	CB	VAL	A1126	-20.074	30.992	36.046	1.00	59.01	A
909	CG1	VAL	A1126	-19.182	30.061	35.194	1.00	60.69	A
910	CG2	VAL	A1126	-21.192	30.053	36.781	1.00	56.87	A
911	C	VAL	A1126	-18.049	32.523	36.642	1.00	56.73	A
912	O	VAL	A1126	-17.828	33.664	36.966	1.00	58.32	A
913	N	SER	A1127	-17.115	31.876	36.004	1.00	56.42	A
914	CA	SER	A1127	-15.795	32.474	35.981	1.00	53.96	A
915	CB	SER	A1127	-15.499	33.164	37.411	1.00	53.65	A
916	OG	SER	A1127	-14.142	33.645	37.645	1.00	53.32	A
917	C	SER	A1127	-14.912	31.249	35.587	1.00	52.67	A
918	O	SER	A1127	-15.029	30.261	36.195	1.00	48.36	A
919	N	PRO	A1128	-14.145	31.335	34.449	1.00	54.07	A
920	CD	PRO	A1128	-14.154	32.579	33.621	1.00	52.53	A
921	CA	PRO	A1128	-13.144	30.401	33.869	1.00	53.71	A
922	CB	PRO	A1128	-12.091	31.369	33.329	1.00	52.36	A
923	CG	PRO	A1128	-12.777	32.972	33.682	1.00	48.45	A
924	C	PRO	A1128	-12.442	29.503	34.925	1.00	55.63	A
925	O	PRO	A1128	-11.473	28.584	34.546	1.00	55.28	A
926	N	ALA	A1129	-12.891	29.792	36.189	1.00	52.77	A
927	CA	ALA	A1129	-12.588	28.993	37.414	1.00	52.53	A
928	CB	ALA	A1129	-11.748	29.794	38.421	1.00	52.73	A
929	C	ALA	A1129	-13.838	28.302	38.089	1.00	52.04	A
930	O	ALA	A1129	-13.673	27.535	38.949	1.00	51.07	A
931	N	GLU	A1130	-15.045	28.566	37.568	1.00	52.56	A
932	CA	GLU	A1130	-16.280	27.987	37.902	1.00	53.76	A
933	CB	GLU	A1130	-17.267	29.130	38.100	1.00	56.22	A
934	CG	GLU	A1130	-16.687	30.513	38.628	1.00	61.14	A
935	CD	GLU	A1130	-16.433	30.690	40.162	1.00	53.08	A
936	OE1	GLU	A1130	-17.344	31.063	40.847	1.00	45.45	A
937	OE2	GLU	A1130	-15.273	30.532	40.616	1.00	57.20	A
938	C	GLU	A1130	-16.880	27.055	36.788	1.00	53.52	A
939	O	GLU	A1130	-18.063	26.678	36.775	1.00	54.66	A

940	N	LYS	A1131	-16.051	26.732	35.816	1.00	52.78	A
941	CA	LYS	A1131	-16.470	26.225	34.535	1.00	49.88	A
942	CB	LYS	A1131	-16.093	27.290	33.506	1.00	47.21	A
943	CG	LYS	A1131	-17.057	27.591	32.218	1.00	51.45	A
944	CD	LYS	A1131	-18.589	28.266	32.338	1.00	43.76	A
945	CE	LYS	A1131	-18.836	29.070	31.014	1.00	48.44	A
946	NZ	LYS	A1131	-18.293	30.582	30.585	1.00	37.94	A
947	C	LYS	A1131	-15.587	24.957	34.452	1.00	49.00	A
948	O	LYS	A1131	-14.321	25.069	34.409	1.00	50.48	A
949	N	TRP	A1132	-16.200	23.792	34.555	1.00	47.26	A
950	CA	TRP	A1132	-15.462	22.542	34.417	1.00	50.44	A
951	CB	TRP	A1132	-15.808	21.648	35.568	1.00	50.76	A
952	CG	TRP	A1132	-15.496	22.268	36.968	1.00	50.73	A
953	CD2	TRP	A1132	-14.317	22.059	37.722	1.00	44.90	A
954	CE2	TRP	A1132	-14.451	22.786	38.904	1.00	48.50	A
955	CE3	TRP	A1132	-13.165	21.306	37.504	1.00	48.73	A
956	CD1	TRP	A1132	-16.329	23.076	37.751	1.00	48.97	A
957	NE1	TRP	A1132	-15.690	23.406	38.886	1.00	46.71	A
958	CZ2	TRP	A1132	-13.463	22.767	39.919	1.00	51.73	A
959	CZ3	TRP	A1132	-12.206	21.298	38.439	1.00	52.00	A
960	CH2	TRP	A1132	-12.353	22.045	39.683	1.00	52.93	A
961	C	TRP	A1132	-15.725	21.749	33.056	1.00	52.06	A
962	O	TRP	A1132	-16.912	21.697	32.549	1.00	51.71	A
963	N	SER	A1133	-14.653	21.191	32.449	1.00	51.83	A
964	CA	SER	A1133	-14.829	20.212	31.345	1.00	54.01	A
965	CB	SER	A1133	-13.844	20.428	30.159	1.00	53.50	A
966	OG	SER	A1133	-14.411	19.675	29.043	1.00	55.87	A
967	C	SER	A1133	-14.933	18.673	31.715	1.00	54.38	A
968	O	SER	A1133	-13.968	18.065	32.411	1.00	57.70	A
969	N	VAL	A1134	-16.004	18.037	31.242	1.00	52.77	A
970	CA	VAL	A1134	-16.173	16.604	31.383	1.00	55.10	A
971	CB	VAL	A1134	-17.510	16.098	30.897	1.00	56.03	A
972	CG1	VAL	A1134	-18.117	15.118	31.965	1.00	51.56	A
973	CG2	VAL	A1134	-18.452	17.284	30.462	1.00	60.83	A
974	C	VAL	A1134	-15.126	15.833	30.633	1.00	54.98	A
975	O	VAL	A1134	-14.668	16.324	29.679	1.00	59.19	A
976	N	HIS	A1135	-14.666	14.714	31.186	1.00	54.51	A
977	CA	HIS	A1135	-13.942	13.626	30.505	1.00	51.51	A
978	CB	HIS	A1135	-12.553	13.703	30.958	1.00	50.38	A
979	CG	HIS	A1135	-11.678	12.696	30.330	1.00	48.22	A
980	CD2	HIS	A1135	-11.901	11.439	29.927	1.00	51.63	A
981	ND1	HIS	A1135	-10.347	12.927	30.105	1.00	48.54	A
982	CE1	HIS	A1135	-9.770	11.840	29.640	1.00	41.81	A
983	NE2	HIS	A1135	-10.692	10.928	29.491	1.00	46.44	A
984	C	HIS	A1135	-14.530	12.208	30.953	1.00	48.59	A
985	O	HIS	A1135	-14.148	11.658	31.887	1.00	51.83	A
986	N	ILE	A1136	-15.536	11.710	30.332	1.00	44.99	A
987	CA	ILE	A1136	-16.240	10.558	30.705	1.00	42.87	A
988	CB	ILE	A1136	-17.179	10.350	29.530	1.00	43.16	A
989	CG2	ILE	A1136	-16.795	9.275	28.721	1.00	45.12	A
990	CG1	ILE	A1136	-18.618	10.358	29.975	1.00	46.38	A
991	CD1	ILE	A1136	-19.272	11.691	29.533	1.00	50.17	A
992	C	ILE	A1136	-15.264	9.391	30.834	1.00	40.23	A
993	O	ILE	A1136	-14.241	9.422	30.248	1.00	39.58	A
994	N	ALA	A1137	-15.526	8.405	31.643	1.00	35.72	A
995	CA	ALA	A1137	-14.465	7.486	31.862	1.00	34.95	A

996	CB	ALA	A1137	-13.438	7.921	32.870	1.00	30.28	A
997	C	ALA	A1137	-15.178	6.131	32.247	1.00	39.24	A
998	O	ALA	A1137	-14.488	5.017	32.531	1.00	39.27	A
999	N	MET	A1138	-16.551	6.185	32.235	1.00	40.82	A
1000	CA	MET	A1138	-17.256	4.861	31.896	1.00	40.07	A
1001	CB	MET	A1138	-18.711	4.725	32.401	1.00	41.41	A
1002	CG	MET	A1138	-19.804	5.478	31.890	1.00	40.93	A
1003	SD	MET	A1138	-19.278	7.165	31.517	1.00	44.96	A
1004	CE	MET	A1138	-20.904	7.656	31.422	1.00	46.83	A
1005	C	MET	A1138	-17.155	4.426	30.518	1.00	41.23	A
1006	O	MET	A1138	-16.519	5.112	29.599	1.00	43.74	A
1007	N	HIS	A1139	-17.859	3.354	30.307	1.00	40.67	A
1008	CA	HIS	A1139	-17.865	2.594	28.956	1.00	42.79	A
1009	CB	HIS	A1139	-18.341	1.038	29.083	1.00	40.32	A
1010	CG	HIS	A1139	-17.948	0.251	27.890	1.00	39.28	A
1011	CD2	HIS	A1139	-16.800	-0.392	27.594	1.00	39.32	A
1012	ND1	HIS	A1139	-18.718	0.222	26.732	1.00	40.16	A
1013	CE1	HIS	A1139	-18.071	-0.444	25.772	1.00	42.03	A
1014	NE2	HIS	A1139	-16.901	-0.825	26.279	1.00	52.16	A
1015	C	HIS	A1139	-18.652	3.457	27.885	1.00	42.45	A
1016	O	HIS	A1139	-19.715	4.072	28.125	1.00	44.34	A
1017	N	PRO	A1140	-18.096	3.669	26.753	1.00	40.56	A
1018	CD	PRO	A1140	-16.972	3.437	25.837	1.00	40.32	A
1019	CA	PRO	A1140	-19.052	4.628	26.224	1.00	39.82	A
1020	CB	PRO	A1140	-18.243	5.339	25.131	1.00	39.97	A
1021	CG	PRO	A1140	-17.028	4.636	24.925	1.00	38.75	A
1022	C	PRO	A1140	-20.274	4.021	25.466	1.00	41.62	A
1023	O	PRO	A1140	-21.085	4.864	24.754	1.00	44.31	A
1024	N	GLN	A1141	-20.464	2.665	25.512	1.00	38.73	A
1025	CA	GLN	A1141	-21.559	2.127	24.669	1.00	38.13	A
1026	CB	GLN	A1141	-21.110	0.979	23.740	1.00	37.92	A
1027	CG	GLN	A1141	-19.477	1.083	23.301	1.00	29.38	A
1028	CD	GLN	A1141	-19.232	0.057	22.227	1.00	35.36	A
1029	OE1	GLN	A1141	-19.186	-1.164	22.440	1.00	40.01	A
1030	NE2	GLN	A1141	-19.351	0.498	21.061	1.00	39.51	A
1031	C	GLN	A1141	-22.752	1.892	25.566	1.00	39.01	A
1032	O	GLN	A1141	-22.547	1.615	26.663	1.00	42.93	A
1033	N	VAL	A1142	-24.000	2.216	25.146	1.00	40.22	A
1034	CA	VAL	A1142	-25.139	2.348	26.044	1.00	37.42	A
1035	CB	VAL	A1142	-25.190	3.804	26.607	1.00	36.84	A
1036	CG1	VAL	A1142	-23.868	4.320	27.478	1.00	28.47	A
1037	CG2	VAL	A1142	-25.542	4.844	25.513	1.00	32.12	A
1038	C	VAL	A1142	-26.407	1.917	25.169	1.00	41.45	A
1039	O	VAL	A1142	-26.376	1.731	23.873	1.00	38.54	A
1040	N	ASN	A1143	-27.493	1.699	25.917	1.00	42.60	A
1041	CA	ASN	A1143	-28.911	1.873	25.387	1.00	45.55	A
1042	CB	ASN	A1143	-29.742	0.680	25.767	1.00	43.97	A
1043	CG	ASN	A1143	-29.237	-0.546	25.032	1.00	45.50	A
1044	OD1	ASN	A1143	-29.357	-1.664	25.549	1.00	40.76	A
1045	ND2	ASN	A1143	-28.606	-0.313	23.823	1.00	35.71	A
1046	C	ASN	A1143	-29.636	3.103	25.859	1.00	45.58	A
1047	O	ASN	A1143	-29.734	3.364	27.050	1.00	46.52	A
1048	N	ILE	A1144	-29.989	3.937	24.940	1.00	45.60	A
1049	CA	ILE	A1144	-30.633	5.128	25.377	1.00	46.25	A
1050	CB	ILE	A1144	-30.435	6.130	24.390	1.00	45.06	A
1051	CG2	ILE	A1144	-31.608	6.974	24.427	1.00	39.54	A

1052	CG1	ILE	A1144	-29.339	7.014	24.755	1.00	50.14	A
1053	CD1	ILE	A1144	-28.081	7.006	23.929	1.00	61.13	A
1054	C	ILE	A1144	-32.175	4.942	25.368	1.00	48.07	A
1055	O	ILE	A1144	-32.754	4.582	24.322	1.00	49.53	A
1056	N	TYR	A1145	-32.816	5.217	26.513	1.00	48.69	A
1057	CA	TYR	A1145	-34.251	5.033	26.766	1.00	48.85	A
1058	CB	TYR	A1145	-34.367	4.256	27.958	1.00	48.27	A
1059	CG	TYR	A1145	-35.730	3.889	28.468	1.00	52.89	A
1060	CD1	TYR	A1145	-36.494	3.030	27.712	1.00	57.74	A
1061	CE1	TYR	A1145	-37.718	2.519	28.176	1.00	53.92	A
1062	CD2	TYR	A1145	-36.165	4.154	29.832	1.00	49.36	A
1063	CE2	TYR	A1145	-37.426	3.661	30.287	1.00	51.26	A
1064	CZ	TYR	A1145	-38.179	2.782	29.416	1.00	53.38	A
1065	OH	TYR	A1145	-39.443	2.143	29.593	1.00	52.73	A
1066	C	TYR	A1145	-34.792	6.431	27.059	1.00	50.45	A
1067	O	TYR	A1145	-33.998	7.409	27.213	1.00	52.93	A
1068	N	SER	A1146	-36.095	6.594	27.037	1.00	49.04	A
1069	CA	SER	A1146	-36.598	7.872	27.290	1.00	49.92	A
1070	CB	SER	A1146	-37.025	8.593	26.022	1.00	49.70	A
1071	OG	SER	A1146	-38.405	8.324	25.813	1.00	51.63	A
1072	C	SER	A1146	-37.830	7.685	28.170	1.00	52.46	A
1073	O	SER	A1146	-38.633	6.716	28.020	1.00	49.79	A
1074	N	VAL	A1147	-38.013	8.676	29.063	1.00	54.45	A
1075	CA	VAL	A1147	-39.024	8.601	30.075	1.00	55.75	A
1076	CB	VAL	A1147	-38.788	9.575	31.024	1.00	55.82	A
1077	CG1	VAL	A1147	-39.326	9.086	32.319	1.00	62.77	A
1078	CG2	VAL	A1147	-37.369	9.700	31.169	1.00	63.13	A
1079	C	VAL	A1147	-40.380	8.940	29.566	1.00	55.24	A
1080	O	VAL	A1147	-41.380	8.563	30.164	1.00	57.12	A
1081	N	THR	A1148	-40.433	9.642	28.465	1.00	55.75	A
1082	CA	THR	A1148	-41.698	10.258	27.987	1.00	55.72	A
1083	CB	THR	A1148	-41.373	11.452	27.035	1.00	55.61	A
1084	OG1	THR	A1148	-40.383	12.325	27.670	1.00	52.66	A
1085	CG2	THR	A1148	-42.661	12.203	26.574	1.00	51.68	A
1086	C	THR	A1148	-42.424	9.093	27.258	1.00	57.84	A
1087	O	THR	A1148	-43.344	8.402	27.866	1.00	56.21	A
1088	N	ARG	A1149	-41.977	8.897	25.991	1.00	56.85	A
1089	CA	ARG	A1149	-42.211	7.635	25.247	1.00	57.81	A
1090	CB	ARG	A1149	-41.430	7.591	23.925	1.00	57.12	A
1091	CG	ARG	A1149	-41.456	8.983	23.212	1.00	63.25	A
1092	CD	ARG	A1149	-43.014	9.356	22.546	1.00	69.05	A
1093	NE	ARG	A1149	-42.813	10.070	21.290	1.00	70.55	A
1094	CZ	ARG	A1149	-42.640	11.387	21.195	1.00	68.20	A
1095	NH1	ARG	A1149	-42.830	12.109	22.335	1.00	60.99	A
1096	NH2	ARG	A1149	-42.252	11.920	19.967	1.00	57.48	A
1097	C	ARG	A1149	-42.142	6.238	25.895	1.00	57.65	A
1098	O	ARG	A1149	-42.743	5.357	25.294	1.00	60.29	A
1099	N	LYS	A1150	-41.400	5.992	26.989	1.00	55.52	A
1100	CA	LYS	A1150	-41.265	4.598	27.551	1.00	53.30	A
1101	CB	LYS	A1150	-42.559	4.133	28.251	1.00	54.72	A
1102	CG	LYS	A1150	-42.723	4.806	29.745	1.00	49.24	A
1103	CD	LYS	A1150	-44.210	4.998	30.178	1.00	52.93	A
1104	CE	LYS	A1150	-44.464	4.112	31.466	1.00	51.43	A
1105	NZ	LYS	A1150	-43.693	2.842	31.275	1.00	53.85	A
1106	C	LYS	A1150	-40.681	3.534	26.673	1.00	52.03	A
1107	O	LYS	A1150	-41.005	2.346	26.807	1.00	50.14	A

1108	N	ARG	A1151	-39.734	3.998	25.811	1.00	53.34	A
1109	CA	ARG	A1151	-39.252	3.360	24.485	1.00	53.49	A
1110	CB	ARG	A1151	-39.997	3.873	23.213	1.00	51.42	A
1111	CG	ARG	A1151	-41.478	3.482	23.222	1.00	49.92	A
1112	CD	ARG	A1151	-41.595	1.862	23.598	1.00	32.45	A
1113	NE	ARG	A1151	-42.978	1.670	23.847	1.00	37.88	A
1114	CZ	ARG	A1151	-43.878	1.562	22.877	1.00	47.36	A
1115	NH1	ARG	A1151	-43.430	1.565	21.567	1.00	38.19	A
1116	NH2	ARG	A1151	-45.239	1.435	23.230	1.00	38.01	A
1117	C	ARG	A1151	-37.787	3.725	24.308	1.00	55.17	A
1118	O	ARG	A1151	-37.342	4.784	24.825	1.00	51.07	A
1119	N	TYR	A1152	-37.095	2.798	23.569	1.00	55.70	A
1120	CA	TYR	A1152	-35.698	2.776	23.282	1.00	54.64	A
1121	CB	TYR	A1152	-35.393	1.333	23.309	1.00	54.61	A
1122	CG	TYR	A1152	-35.141	0.900	24.708	1.00	58.49	A
1123	CD1	TYR	A1152	-36.132	0.280	25.429	1.00	55.61	A
1124	CE1	TYR	A1152	-35.914	-0.121	26.688	1.00	49.92	A
1125	CD2	TYR	A1152	-33.936	1.263	25.418	1.00	57.22	A
1126	CE2	TYR	A1152	-33.770	0.827	26.798	1.00	47.70	A
1127	CZ	TYR	A1152	-34.748	0.156	27.353	1.00	47.04	A
1128	OH	TYR	A1152	-34.690	-0.235	28.656	1.00	56.25	A
1129	C	TYR	A1152	-35.268	3.287	21.906	1.00	55.84	A
1130	O	TYR	A1152	-35.774	2.847	20.881	1.00	56.67	A
1131	N	ALA	A1153	-34.245	4.144	21.887	1.00	56.59	A
1132	CA	ALA	A1153	-33.760	4.832	20.732	1.00	55.99	A
1133	CB	ALA	A1153	-32.783	6.005	21.159	1.00	56.07	A
1134	C	ALA	A1153	-33.006	3.839	19.955	1.00	56.92	A
1135	O	ALA	A1153	-32.571	2.897	20.469	1.00	57.30	A
1136	N	HIS	A1154	-32.808	4.115	18.674	1.00	60.67	A
1137	CA	HIS	A1154	-31.980	3.237	17.781	1.00	61.19	A
1138	CB	HIS	A1154	-32.509	1.819	17.795	1.00	62.05	A
1139	CG	HIS	A1154	-33.888	1.769	17.278	1.00	64.88	A
1140	CD2	HIS	A1154	-34.502	0.909	16.429	1.00	71.23	A
1141	ND1	HIS	A1154	-34.810	2.719	17.639	1.00	67.70	A
1142	CE1	HIS	A1154	-35.961	2.418	17.051	1.00	80.44	A
1143	NE2	HIS	A1154	-35.798	1.329	16.301	1.00	78.35	A
1144	C	HIS	A1154	-32.241	3.637	16.353	1.00	58.30	A
1145	O	HIS	A1154	-33.111	4.457	16.139	1.00	55.10	A
1146	N	LEU	A1155	-31.563	2.900	15.439	1.00	57.17	A
1147	CA	LEU	A1155	-31.470	3.175	13.990	1.00	55.23	A
1148	CB	LEU	A1155	-30.212	2.553	13.423	1.00	55.99	A
1149	CG	LEU	A1155	-29.912	2.535	11.908	1.00	56.61	A
1150	CD1	LEU	A1155	-29.517	4.092	11.605	1.00	51.06	A
1151	CD2	LEU	A1155	-28.826	1.329	11.342	1.00	44.95	A
1152	C	LEU	A1155	-32.752	2.711	13.300	1.00	57.81	A
1153	O	LEU	A1155	-33.362	1.627	13.647	1.00	57.77	A
1154	N	SER	A1156	-33.195	3.610	12.409	1.00	58.62	A
1155	CA	SER	A1156	-34.488	3.599	11.720	1.00	57.48	A
1156	CB	SER	A1156	-34.700	4.997	11.079	1.00	57.42	A
1157	OG	SER	A1156	-36.082	5.267	10.670	1.00	56.33	A
1158	C	SER	A1156	-34.493	2.524	10.642	1.00	58.57	A
1159	O	SER	A1156	-33.451	1.907	10.362	1.00	56.39	A
1160	N	ALA	A1157	-35.650	2.430	9.941	1.00	62.16	A
1161	CA	ALA	A1157	-36.087	1.258	9.172	1.00	63.89	A
1162	CB	ALA	A1157	-37.416	0.797	9.731	1.00	63.50	A
1163	C	ALA	A1157	-36.150	1.504	7.630	1.00	66.42	A

1164	O	ALA	A1157	-35.105	1.555	6.904	1.00	66.46	A
1165	N	ARG	A1158	-37.377	1.652	7.130	1.00	67.87	A
1166	CA	ARG	A1158	-37.619	2.097	5.716	1.00	67.26	A
1167	CB	ARG	A1158	-39.040	1.720	5.228	1.00	66.92	A
1168	CG	ARG	A1158	-39.490	0.194	5.229	1.00	69.49	A
1169	CD	ARG	A1158	-38.660	-0.806	4.374	1.00	70.89	A
1170	NE	ARG	A1158	-39.456	-2.015	4.025	1.00	66.35	A
1171	CZ	ARG	A1158	-38.945	-3.153	3.489	1.00	65.67	A
1172	NH1	ARG	A1158	-37.641	-3.309	3.203	1.00	62.24	A
1173	NH2	ARG	A1158	-39.735	-4.176	3.223	1.00	63.92	A
1174	C	ARG	A1158	-37.418	3.639	5.774	1.00	64.75	A
1175	O	ARG	A1158	-36.524	4.218	5.119	1.00	65.92	A
1176	N	PRO	A1159	-38.060	4.259	6.738	1.00	61.37	A
1177	CD	PRO	A1159	-38.882	3.757	7.818	1.00	61.45	A
1178	CA	PRO	A1159	-37.718	5.626	6.983	1.00	60.77	A
1179	CB	PRO	A1159	-38.681	5.997	8.114	1.00	60.75	A
1180	CG	PRO	A1159	-39.680	4.969	8.240	1.00	56.17	A
1181	C	PRO	A1159	-36.237	5.673	7.588	1.00	61.31	A
1182	O	PRO	A1159	-35.941	6.684	8.318	1.00	57.51	A
1183	N	ALA	A1160	-35.389	4.595	7.356	1.00	59.83	A
1184	CA	ALA	A1160	-33.987	4.635	7.826	1.00	60.22	A
1185	CB	ALA	A1160	-33.096	3.757	6.921	1.00	62.60	A
1186	C	ALA	A1160	-33.464	6.148	7.899	1.00	60.09	A
1187	O	ALA	A1160	-34.285	7.072	7.957	1.00	58.25	A
1188	N	ASP	A1161	-32.144	6.384	7.751	1.00	58.76	A
1189	CA	ASP	A1161	-31.508	7.701	7.975	1.00	57.33	A
1190	CB	ASP	A1161	-31.807	8.701	6.889	1.00	56.95	A
1191	CG	ASP	A1161	-30.681	9.841	6.809	1.00	60.13	A
1192	OD1	ASP	A1161	-29.529	9.464	6.366	1.00	61.49	A
1193	OD2	ASP	A1161	-30.929	11.047	7.250	1.00	57.19	A
1194	C	ASP	A1161	-31.746	8.412	9.339	1.00	55.49	A
1195	O	ASP	A1161	-31.079	9.356	9.686	1.00	54.97	A
1196	N	GLU	A1162	-32.723	7.984	10.090	1.00	55.55	A
1197	CA	GLU	A1162	-33.100	8.741	11.288	1.00	56.05	A
1198	CB	GLU	A1162	-34.553	9.233	11.191	1.00	53.04	A
1199	CG	GLU	A1162	-35.363	8.090	11.562	1.00	57.50	A
1200	CD	GLU	A1162	-36.885	8.199	11.483	1.00	60.84	A
1201	OE1	GLU	A1162	-37.623	7.086	11.415	1.00	48.37	A
1202	OE2	GLU	A1162	-37.283	9.392	11.523	1.00	61.98	A
1203	C	GLU	A1162	-32.894	7.638	12.425	1.00	56.30	A
1204	O	GLU	A1162	-33.069	6.345	12.132	1.00	54.69	A
1205	N	ILE	A1163	-32.488	8.118	13.635	1.00	53.87	A
1206	CA	ILE	A1163	-32.674	7.310	14.885	1.00	52.76	A
1207	CB	ILE	A1163	-31.704	7.727	16.054	1.00	53.12	A
1208	CG2	ILE	A1163	-31.859	6.808	17.364	1.00	53.60	A
1209	CG1	ILE	A1163	-30.259	7.554	15.603	1.00	57.71	A
1210	CD1	ILE	A1163	-29.194	8.356	16.468	1.00	55.58	A
1211	C	ILE	A1163	-34.009	7.501	15.465	1.00	49.76	A
1212	O	ILE	A1163	-34.261	8.523	15.979	1.00	49.36	A
1213	N	ALA	A1164	-34.854	6.482	15.500	1.00	50.56	A
1214	CA	ALA	A1164	-36.054	6.544	16.330	1.00	50.15	A
1215	CB	ALA	A1164	-37.205	5.844	15.609	1.00	46.07	A
1216	C	ALA	A1164	-35.881	6.050	17.849	1.00	51.94	A
1217	O	ALA	A1164	-34.744	5.874	18.357	1.00	52.54	A
1218	N	VAL	A1165	-37.036	5.713	18.466	1.00	53.57	A
1219	CA	VAL	A1165	-37.253	5.301	19.768	1.00	53.73	A

1220	CB	VAL	A1165	-37.705	6.578	20.550	1.00	56.97	A
1221	CG1	VAL	A1165	-36.488	7.685	21.122	1.00	51.57	A
1222	CG2	VAL	A1165	-38.761	7.281	19.596	1.00	55.96	A
1223	C	VAL	A1165	-38.592	4.507	19.654	1.00	54.88	A
1224	O	VAL	A1165	-39.596	4.960	20.272	1.00	56.25	A
1225	N	ASP	A1166	-38.721	3.338	18.991	1.00	53.54	A
1226	CA	ASP	A1166	-40.016	2.702	19.183	1.00	51.08	A
1227	CB	ASP	A1166	-40.970	3.054	18.101	1.00	50.65	A
1228	CG	ASP	A1166	-40.262	3.252	16.714	1.00	56.08	A
1229	OD1	ASP	A1166	-39.803	4.346	16.406	1.00	53.36	A
1230	OD2	ASP	A1166	-40.033	2.246	15.919	1.00	71.03	A
1231	C	ASP	A1166	-39.918	1.222	19.378	1.00	55.17	A
1232	O	ASP	A1166	-40.338	0.404	18.366	1.00	54.94	A
1233	N	ARG	A1167	-39.442	0.828	20.643	1.00	53.75	A
1234	CA	ARG	A1167	-39.323	-0.531	21.017	1.00	54.81	A
1235	CB	ARG	A1167	-38.137	-1.115	20.228	1.00	56.32	A
1236	CG	ARG	A1167	-36.723	-0.390	20.364	1.00	58.78	A
1237	CD	ARG	A1167	-35.681	-0.506	19.040	1.00	56.26	A
1238	NE	ARG	A1167	-35.475	-1.913	18.687	1.00	66.10	A
1239	CZ	ARG	A1167	-34.425	-2.475	18.055	1.00	64.26	A
1240	NH1	ARG	A1167	-33.380	-1.791	17.648	1.00	67.66	A
1241	NH2	ARG	A1167	-34.398	-3.774	17.824	1.00	63.32	A
1242	C	ARG	A1167	-39.143	-0.855	22.488	1.00	57.24	A
1243	O	ARG	A1167	-38.271	-0.342	23.165	1.00	61.82	A
1244	N	ASP	A1168	-39.903	-1.774	23.014	1.00	56.05	A
1245	CA	ASP	A1168	-40.062	-1.945	24.388	1.00	53.81	A
1246	CB	ASP	A1168	-41.285	-2.903	24.430	1.00	53.85	A
1247	CG	ASP	A1168	-42.126	-2.857	25.745	1.00	57.19	A
1248	OD1	ASP	A1168	-42.801	-1.756	26.147	1.00	47.73	A
1249	OD2	ASP	A1168	-42.122	-4.031	26.301	1.00	55.70	A
1250	C	ASP	A1168	-38.814	-2.700	24.818	1.00	56.17	A
1251	O	ASP	A1168	-38.709	-3.252	26.003	1.00	60.36	A
1252	N	VAL	A1169	-37.879	-2.937	23.908	1.00	53.28	A
1253	CA	VAL	A1169	-36.672	-3.515	24.392	1.00	51.53	A
1254	CB	VAL	A1169	-36.813	-4.995	24.750	1.00	51.11	A
1255	CG1	VAL	A1169	-36.501	-5.926	23.476	1.00	52.93	A
1256	CG2	VAL	A1169	-35.893	-5.410	26.028	1.00	47.17	A
1257	C	VAL	A1169	-35.762	-3.172	23.292	1.00	53.59	A
1258	O	VAL	A1169	-36.141	-3.222	22.146	1.00	57.16	A
1259	N	PRO	A1170	-34.558	-2.753	23.592	1.00	53.16	A
1260	CD	PRO	A1170	-34.002	-2.555	24.924	1.00	55.06	A
1261	CA	PRO	A1170	-33.574	-2.548	22.565	1.00	50.23	A
1262	CB	PRO	A1170	-32.424	-1.930	23.373	1.00	51.03	A
1263	CG	PRO	A1170	-32.495	-2.584	24.678	1.00	51.68	A
1264	C	PRO	A1170	-32.991	-3.852	21.997	1.00	50.54	A
1265	O	PRO	A1170	-31.966	-4.328	22.595	1.00	51.10	A
1266	N	TRP	A1171	-33.529	-4.459	20.900	1.00	45.96	A
1267	CA	TRP	A1171	-32.870	-5.767	20.463	1.00	43.27	A
1268	CB	TRP	A1171	-33.932	-6.850	20.228	1.00	43.79	A
1269	CG	TRP	A1171	-33.724	-8.187	20.789	1.00	35.64	A
1270	CD2	TRP	A1171	-33.597	-8.511	22.178	1.00	31.83	A
1271	CE2	TRP	A1171	-33.369	-9.859	22.297	1.00	29.18	A
1272	CE3	TRP	A1171	-33.823	-7.775	23.371	1.00	43.31	A
1273	CD1	TRP	A1171	-33.501	-9.278	20.105	1.00	38.83	A
1274	NE1	TRP	A1171	-33.141	-10.331	21.056	1.00	40.85	A
1275	CZ2	TRP	A1171	-33.258	-10.498	23.555	1.00	44.74	A

1276	CZ3	TRP	A1171	-33.765	-8.433	24.695	1.00	38.91	A
1277	CH2	TRP	A1171	-33.408	-9.744	24.764	1.00	39.03	A
1278	C	TRP	A1171	-31.959	-5.488	19.253	1.00	42.02	A
1279	O	TRP	A1171	-32.127	-4.373	18.652	1.00	45.51	A
1280	N	GLY	A1172	-30.956	-6.333	18.988	1.00	37.21	A
1281	CA	GLY	A1172	-29.812	-6.174	18.123	1.00	36.44	A
1282	C	GLY	A1172	-29.299	-4.772	17.737	1.00	42.21	A
1283	O	GLY	A1172	-29.577	-3.745	18.389	1.00	44.18	A
1284	N	VAL	A1173	-28.594	-4.694	16.582	1.00	45.05	A
1285	CA	VAL	A1173	-27.714	-3.607	16.230	1.00	44.26	A
1286	CB	VAL	A1173	-26.944	-3.782	14.904	1.00	43.11	A
1287	CG1	VAL	A1173	-25.435	-4.042	15.206	1.00	39.57	A
1288	CG2	VAL	A1173	-27.614	-4.542	13.733	1.00	33.62	A
1289	C	VAL	A1173	-28.261	-2.187	16.097	1.00	47.76	A
1290	O	VAL	A1173	-27.537	-1.241	15.702	1.00	51.06	A
1291	N	ASP	A1174	-29.515	-1.998	16.332	1.00	47.47	A
1292	CA	ASP	A1174	-30.133	-0.779	15.902	1.00	49.07	A
1293	CB	ASP	A1174	-31.574	-1.150	15.516	1.00	47.81	A
1294	CG	ASP	A1174	-31.628	-2.586	15.080	1.00	53.25	A
1295	OD1	ASP	A1174	-30.935	-2.924	14.062	1.00	62.21	A
1296	OD2	ASP	A1174	-32.206	-3.407	15.798	1.00	52.20	A
1297	C	ASP	A1174	-30.135	-0.004	17.198	1.00	48.59	A
1298	O	ASP	A1174	-30.478	1.133	17.261	1.00	51.13	A
1299	N	SER	A1175	-29.852	-0.688	18.260	1.00	45.38	A
1300	CA	SER	A1175	-30.133	-0.188	19.460	1.00	43.01	A
1301	CB	SER	A1175	-30.520	-1.373	20.232	1.00	44.33	A
1302	OG	SER	A1175	-31.937	-1.451	20.312	1.00	46.67	A
1303	C	SER	A1175	-28.902	0.466	19.953	1.00	42.69	A
1304	O	SER	A1175	-29.040	1.445	20.561	1.00	47.61	A
1305	N	LEU	A1176	-27.703	0.085	19.576	1.00	43.34	A
1306	CA	LEU	A1176	-26.442	0.465	20.168	1.00	42.70	A
1307	CB	LEU	A1176	-25.389	-0.608	19.891	1.00	44.56	A
1308	CG	LEU	A1176	-23.927	-0.343	20.407	1.00	40.80	A
1309	CD1	LEU	A1176	-23.785	-0.914	21.682	1.00	28.04	A
1310	CD2	LEU	A1176	-22.824	-0.991	19.531	1.00	38.35	A
1311	C	LEU	A1176	-25.787	1.727	19.727	1.00	44.08	A
1312	O	LEU	A1176	-25.293	1.851	18.547	1.00	44.75	A
1313	N	ILE	A1177	-25.606	2.576	20.736	1.00	42.42	A
1314	CA	ILE	A1177	-25.150	3.921	20.587	1.00	41.76	A
1315	CB	ILE	A1177	-26.272	4.811	21.284	1.00	42.87	A
1316	CG2	ILE	A1177	-25.818	6.326	21.517	1.00	41.23	A
1317	CG1	ILE	A1177	-27.518	4.705	20.380	1.00	41.14	A
1318	CD1	ILE	A1177	-28.729	5.595	20.689	1.00	41.52	A
1319	C	ILE	A1177	-23.799	4.168	21.234	1.00	42.23	A
1320	O	ILE	A1177	-23.518	3.608	22.280	1.00	47.69	A
1321	N	THR	A1178	-23.003	5.073	20.753	1.00	41.58	A
1322	CA	THR	A1178	-21.655	5.301	21.313	1.00	42.66	A
1323	CB	THR	A1178	-20.328	4.631	20.482	1.00	43.24	A
1324	OG1	THR	A1178	-20.366	3.207	20.512	1.00	45.69	A
1325	CG2	THR	A1178	-18.929	4.906	20.981	1.00	39.91	A
1326	C	THR	A1178	-21.531	6.774	21.629	1.00	45.89	A
1327	O	THR	A1178	-21.653	7.713	20.766	1.00	42.36	A
1328	N	LEU	A1179	-21.240	6.982	22.950	1.00	48.42	A
1329	CA	LEU	A1179	-21.004	8.294	23.365	1.00	48.14	A
1330	CB	LEU	A1179	-21.345	8.420	24.764	1.00	45.95	A
1331	CG	LEU	A1179	-22.819	8.159	25.043	1.00	47.99	A

1332	CD1	LEU	A1179	-23.042	8.398	26.645	1.00	50.10	A
1333	CD2	LEU	A1179	-23.847	9.013	24.322	1.00	36.60	A
1334	C	LEU	A1179	-19.555	8.477	23.028	1.00	50.76	A
1335	O	LEU	A1179	-18.663	8.406	23.895	1.00	54.63	A
1336	N	ALA	A1180	-19.277	8.705	21.739	1.00	51.61	A
1337	CA	ALA	A1180	-17.870	9.024	21.388	1.00	52.29	A
1338	CB	ALA	A1180	-17.609	8.850	19.960	1.00	51.30	A
1339	C	ALA	A1180	-17.449	10.476	21.825	1.00	51.43	A
1340	O	ALA	A1180	-18.245	11.278	22.107	1.00	48.12	A
1341	N	PHE	A1181	-16.151	10.718	21.884	1.00	54.36	A
1342	CA	PHE	A1181	-15.582	12.021	22.014	1.00	55.65	A
1343	CB	PHE	A1181	-14.106	11.896	22.295	1.00	55.80	A
1344	CG	PHE	A1181	-13.740	11.072	23.434	1.00	52.74	A
1345	CD1	PHE	A1181	-14.096	11.447	24.725	1.00	53.31	A
1346	CD2	PHE	A1181	-12.856	10.013	23.264	1.00	54.49	A
1347	CE1	PHE	A1181	-13.609	10.759	25.919	1.00	49.29	A
1348	CE2	PHE	A1181	-12.393	9.206	24.445	1.00	43.68	A
1349	CZ	PHE	A1181	-12.810	9.620	25.734	1.00	55.56	A
1350	C	PHE	A1181	-15.619	12.807	20.730	1.00	58.19	A
1351	O	PHE	A1181	-15.921	12.342	19.589	1.00	59.27	A
1352	N	GLN	A1182	-15.119	13.992	20.948	1.00	59.83	A
1353	CA	GLN	A1182	-15.404	15.188	20.177	1.00	63.20	A
1354	CB	GLN	A1182	-16.958	15.520	19.992	1.00	60.39	A
1355	CG	GLN	A1182	-17.263	15.527	18.434	1.00	68.90	A
1356	CD	GLN	A1182	-18.416	16.452	17.773	1.00	69.42	A
1357	OE1	GLN	A1182	-18.719	17.578	18.210	1.00	81.45	A
1358	NE2	GLN	A1182	-19.011	15.946	16.716	1.00	71.57	A
1359	C	GLN	A1182	-14.558	16.263	20.959	1.00	61.62	A
1360	O	GLN	A1182	-13.406	16.035	21.392	1.00	61.76	A
1361	N	ASP	A1183	-15.083	17.430	21.139	1.00	60.93	A
1362	CA	ASP	A1183	-14.176	18.413	21.586	1.00	62.18	A
1363	CB	ASP	A1183	-13.604	19.312	20.452	1.00	61.58	A
1364	CG	ASP	A1183	-14.671	19.682	19.333	1.00	63.90	A
1365	OD1	ASP	A1183	-15.793	20.241	19.690	1.00	61.47	A
1366	OD2	ASP	A1183	-14.336	19.418	18.099	1.00	61.93	A
1367	C	ASP	A1183	-14.970	19.078	22.683	1.00	62.92	A
1368	O	ASP	A1183	-15.812	20.014	22.443	1.00	62.62	A
1369	N	GLN	A1184	-14.742	18.456	23.876	1.00	60.93	A
1370	CA	GLN	A1184	-15.360	18.890	25.112	1.00	59.39	A
1371	CB	GLN	A1184	-15.045	20.419	25.457	1.00	58.37	A
1372	CG	GLN	A1184	-13.422	20.721	25.438	1.00	59.71	A
1373	CD	GLN	A1184	-12.484	19.349	25.450	1.00	63.12	A
1374	OE1	GLN	A1184	-12.634	18.412	26.340	1.00	68.29	A
1375	NE2	GLN	A1184	-11.539	19.255	24.488	1.00	51.48	A
1376	C	GLN	A1184	-16.741	18.565	24.709	1.00	58.21	A
1377	O	GLN	A1184	-17.747	19.225	24.980	1.00	60.69	A
1378	N	ARG	A1185	-16.835	17.545	23.945	1.00	55.63	A
1379	CA	ARG	A1185	-18.206	17.350	23.532	1.00	54.81	A
1380	CB	ARG	A1185	-18.549	18.370	22.438	1.00	53.90	A
1381	CG	ARG	A1185	-19.202	19.725	22.998	1.00	56.94	A
1382	CD	ARG	A1185	-20.234	20.450	21.838	1.00	55.54	A
1383	NE	ARG	A1185	-20.678	21.761	22.186	1.00	52.09	A
1384	CZ	ARG	A1185	-21.757	22.000	22.949	1.00	55.77	A
1385	NH1	ARG	A1185	-22.597	21.005	23.277	1.00	55.38	A
1386	NH2	ARG	A1185	-22.087	23.281	23.295	1.00	52.30	A
1387	C	ARG	A1185	-18.491	15.868	23.198	1.00	52.14	A

1388	O	ARG	A1185	-17.543	15.060	23.014	1.00	47.69	A
1389	N	TYR	A1186	-19.767	15.490	23.126	1.00	49.53	A
1390	CA	TYR	A1186	-19.987	14.031	22.848	1.00	48.90	A
1391	CB	TYR	A1186	-20.145	13.344	24.188	1.00	49.15	A
1392	CG	TYR	A1186	-18.960	13.360	25.180	1.00	43.95	A
1393	CD1	TYR	A1186	-17.991	12.478	25.050	1.00	38.49	A
1394	CE1	TYR	A1186	-16.933	12.363	25.867	1.00	45.67	A
1395	CD2	TYR	A1186	-18.933	14.163	26.272	1.00	46.78	A
1396	CE2	TYR	A1186	-17.857	14.048	27.243	1.00	53.74	A
1397	CZ	TYR	A1186	-16.853	13.113	26.976	1.00	52.64	A
1398	OH	TYR	A1186	-15.789	12.923	27.730	1.00	49.85	A
1399	C	TYR	A1186	-21.167	13.638	21.885	1.00	51.68	A
1400	O	TYR	A1186	-22.415	13.576	22.295	1.00	53.77	A
1401	N	SER	A1187	-20.874	13.370	20.607	1.00	51.07	A
1402	CA	SER	A1187	-21.949	12.821	19.698	1.00	50.53	A
1403	CB	SER	A1187	-21.509	12.842	18.256	1.00	50.97	A
1404	OG	SER	A1187	-20.240	12.399	18.196	1.00	46.43	A
1405	C	SER	A1187	-22.468	11.420	19.902	1.00	50.50	A
1406	O	SER	A1187	-21.768	10.518	20.051	1.00	53.19	A
1407	N	VAL	A1188	-23.730	11.244	19.900	1.00	49.79	A
1408	CA	VAL	A1188	-24.264	9.950	19.660	1.00	50.91	A
1409	CB	VAL	A1188	-25.768	10.067	19.982	1.00	53.23	A
1410	CG1	VAL	A1188	-25.910	10.318	21.545	1.00	47.80	A
1411	CG2	VAL	A1188	-26.384	11.324	19.273	1.00	54.19	A
1412	C	VAL	A1188	-23.983	9.255	18.287	1.00	51.02	A
1413	O	VAL	A1188	-24.601	9.469	17.215	1.00	52.30	A
1414	N	GLN	A1189	-23.031	8.381	18.340	1.00	51.11	A
1415	CA	GLN	A1189	-22.589	7.730	17.164	1.00	51.01	A
1416	CB	GLN	A1189	-21.104	7.314	17.179	1.00	50.24	A
1417	CG	GLN	A1189	-20.700	6.676	15.832	1.00	40.12	A
1418	CD	GLN	A1189	-19.217	6.617	15.776	1.00	48.75	A
1419	OE1	GLN	A1189	-18.633	6.927	14.663	1.00	41.63	A
1420	NE2	GLN	A1189	-18.500	6.314	17.055	1.00	39.82	A
1421	C	GLN	A1189	-23.253	6.430	17.172	1.00	51.60	A
1422	O	GLN	A1189	-23.268	5.773	18.202	1.00	52.55	A
1423	N	THR	A1190	-23.568	5.990	15.947	1.00	49.64	A
1424	CA	THR	A1190	-24.546	4.967	15.749	1.00	45.96	A
1425	CB	THR	A1190	-25.375	5.475	14.541	1.00	44.37	A
1426	OG1	THR	A1190	-24.538	6.391	13.854	1.00	43.61	A
1427	CG2	THR	A1190	-26.390	6.228	15.074	1.00	45.56	A
1428	C	THR	A1190	-23.787	3.693	15.497	1.00	41.56	A
1429	O	THR	A1190	-22.656	3.815	15.348	1.00	38.29	A
1430	N	ALA	A1191	-24.430	2.555	15.246	1.00	42.07	A
1431	CA	ALA	A1191	-23.701	1.286	14.972	1.00	45.40	A
1432	CB	ALA	A1191	-24.487	0.021	15.338	1.00	43.33	A
1433	C	ALA	A1191	-23.098	1.100	13.614	1.00	47.54	A
1434	O	ALA	A1191	-22.289	0.169	13.501	1.00	48.25	A
1435	N	ASP	A1192	-23.510	1.919	12.639	1.00	48.63	A
1436	CA	ASP	A1192	-22.907	1.988	11.308	1.00	49.53	A
1437	CB	ASP	A1192	-23.995	2.171	10.258	1.00	52.00	A
1438	CG	ASP	A1192	-24.994	3.411	10.562	1.00	56.24	A
1439	OD1	ASP	A1192	-24.748	4.155	11.561	1.00	60.73	A
1440	OD2	ASP	A1192	-25.978	3.619	9.776	1.00	52.99	A
1441	C	ASP	A1192	-21.920	3.141	11.136	1.00	49.08	A
1442	O	ASP	A1192	-21.324	3.325	10.039	1.00	49.27	A
1443	N	HIS	A1193	-21.685	3.886	12.195	1.00	48.30	A

1444	CA	HIS	A1193	-20.533	4.838	12.314	1.00	47.88	A
1445	CB	HIS	A1193	-19.599	4.636	11.211	1.00	48.10	A
1446	CG	HIS	A1193	-18.775	3.443	11.386	1.00	48.11	A
1447	CD2	HIS	A1193	-17.577	3.111	10.915	1.00	46.17	A
1448	ND1	HIS	A1193	-19.156	2.421	12.207	1.00	56.60	A
1449	CE1	HIS	A1193	-18.258	1.462	12.161	1.00	49.47	A
1450	NE2	HIS	A1193	-17.266	1.893	11.441	1.00	46.34	A
1451	C	HIS	A1193	-20.927	6.311	12.233	1.00	49.66	A
1452	O	HIS	A1193	-20.086	7.236	12.346	1.00	52.17	A
1453	N	ARG	A1194	-22.183	6.573	12.041	1.00	49.16	A
1454	CA	ARG	A1194	-22.456	7.896	11.699	1.00	50.30	A
1455	CB	ARG	A1194	-23.584	7.971	10.625	1.00	54.54	A
1456	CG	ARG	A1194	-23.608	7.074	9.301	1.00	49.25	A
1457	CD	ARG	A1194	-24.944	7.273	8.725	1.00	45.22	A
1458	NE	ARG	A1194	-25.729	6.082	8.994	1.00	50.21	A
1459	CZ	ARG	A1194	-26.957	5.903	8.472	1.00	54.72	A
1460	NH1	ARG	A1194	-27.474	6.917	7.787	1.00	55.93	A
1461	NH2	ARG	A1194	-27.683	4.764	8.621	1.00	52.24	A
1462	C	ARG	A1194	-23.028	8.533	12.965	1.00	51.72	A
1463	O	ARG	A1194	-23.289	7.858	13.971	1.00	53.54	A
1464	N	PHE	A1195	-23.261	9.831	12.893	1.00	51.55	A
1465	CA	PHE	A1195	-23.519	10.617	14.081	1.00	51.97	A
1466	CB	PHE	A1195	-22.474	11.676	14.373	1.00	47.85	A
1467	CG	PHE	A1195	-21.013	11.177	14.338	1.00	47.97	A
1468	CD1	PHE	A1195	-20.260	11.207	13.125	1.00	45.55	A
1469	CD2	PHE	A1195	-20.339	10.826	15.539	1.00	40.06	A
1470	CE1	PHE	A1195	-18.879	10.886	13.141	1.00	51.26	A
1471	CE2	PHE	A1195	-18.986	10.415	15.563	1.00	44.02	A
1472	CZ	PHE	A1195	-18.222	10.401	14.389	1.00	43.72	A
1473	C	PHE	A1195	-24.951	11.170	13.993	1.00	53.19	A
1474	O	PHE	A1195	-25.619	10.990	12.947	1.00	51.90	A
1475	N	LEU	A1196	-25.472	11.716	15.120	1.00	53.01	A
1476	CA	LEU	A1196	-26.740	12.504	14.967	1.00	54.25	A
1477	CB	LEU	A1196	-27.686	12.081	16.075	1.00	53.91	A
1478	CG	LEU	A1196	-29.158	12.444	16.241	1.00	51.72	A
1479	CD1	LEU	A1196	-30.107	11.568	15.518	1.00	46.79	A
1480	CD2	LEU	A1196	-29.485	12.313	17.653	1.00	52.55	A
1481	C	LEU	A1196	-26.646	14.089	14.786	1.00	54.79	A
1482	O	LEU	A1196	-26.526	14.815	15.694	1.00	55.60	A
1483	N	ARG	A1197	-26.674	14.653	13.620	1.00	57.25	A
1484	CA	ARG	A1197	-26.525	16.093	13.649	1.00	59.59	A
1485	CB	ARG	A1197	-26.770	16.698	12.236	1.00	61.90	A
1486	CG	ARG	A1197	-26.635	18.274	12.041	1.00	60.84	A
1487	CD	ARG	A1197	-26.532	18.411	10.551	1.00	61.17	A
1488	NE	ARG	A1197	-25.521	17.447	10.129	1.00	71.05	A
1489	CZ	ARG	A1197	-24.355	17.727	9.521	1.00	71.31	A
1490	NH1	ARG	A1197	-24.050	18.970	9.183	1.00	71.86	A
1491	NH2	ARG	A1197	-23.495	16.746	9.220	1.00	72.37	A
1492	C	ARG	A1197	-27.574	16.639	14.601	1.00	59.05	A
1493	O	ARG	A1197	-28.801	16.248	14.608	1.00	60.61	A
1494	N	HIS	A1198	-27.103	17.496	15.461	1.00	57.90	A
1495	CA	HIS	A1198	-28.062	18.256	16.292	1.00	57.50	A
1496	CB	HIS	A1198	-27.381	19.519	16.848	1.00	57.78	A
1497	CG	HIS	A1198	-27.875	20.801	16.299	1.00	58.21	A
1498	CD2	HIS	A1198	-29.123	21.327	16.204	1.00	57.81	A
1499	ND1	HIS	A1198	-27.009	21.750	15.793	1.00	61.93	A

1500	CE1	HIS	A1198	-27.707	22.815	15.425	1.00	56.68	A
1501	NE2	HIS	A1198	-28.986	22.579	15.677	1.00	56.90	A
1502	C	HIS	A1198	-29.373	18.464	15.521	1.00	55.84	A
1503	O	HIS	A1198	-30.474	18.275	16.097	1.00	55.29	A
1504	N	ASP	A1199	-29.250	18.621	14.198	1.00	55.33	A
1505	CA	ASP	A1199	-30.504	18.786	13.300	1.00	56.82	A
1506	CB	ASP	A1199	-30.241	19.132	11.795	1.00	57.28	A
1507	CG	ASP	A1199	-30.022	17.905	10.978	1.00	65.11	A
1508	OD1	ASP	A1199	-31.067	17.408	10.423	1.00	73.36	A
1509	OD2	ASP	A1199	-28.842	17.421	10.883	1.00	63.85	A
1510	C	ASP	A1199	-31.588	17.735	13.369	1.00	53.76	A
1511	O	ASP	A1199	-32.735	18.113	13.724	1.00	51.71	A
1512	N	GLY	A1200	-31.253	16.434	13.145	1.00	52.48	A
1513	CA	GLY	A1200	-32.309	15.383	13.271	1.00	53.35	A
1514	C	GLY	A1200	-31.821	14.263	12.443	1.00	57.34	A
1515	O	GLY	A1200	-32.587	13.247	12.142	1.00	58.17	A
1516	N	ARG	A1201	-30.526	14.424	12.070	1.00	58.58	A
1517	CA	ARG	A1201	-29.948	13.738	10.895	1.00	61.02	A
1518	CB	ARG	A1201	-29.876	14.699	9.716	1.00	58.55	A
1519	CG	ARG	A1201	-30.977	14.510	8.638	1.00	67.94	A
1520	CD	ARG	A1201	-30.594	15.246	7.136	1.00	68.54	A
1521	NE	ARG	A1201	-29.927	16.616	7.315	1.00	75.23	A
1522	CZ	ARG	A1201	-28.594	16.879	7.413	1.00	64.57	A
1523	NH1	ARG	A1201	-28.148	18.121	7.508	1.00	57.11	A
1524	NH2	ARG	A1201	-27.714	15.887	7.380	1.00	67.34	A
1525	C	ARG	A1201	-28.549	13.204	11.142	1.00	60.11	A
1526	O	ARG	A1201	-27.547	13.974	11.322	1.00	57.48	A
1527	N	LEU	A1202	-28.482	11.864	11.138	1.00	59.21	A
1528	CA	LEU	A1202	-27.194	11.167	11.058	1.00	54.32	A
1529	CB	LEU	A1202	-27.479	9.667	11.240	1.00	53.92	A
1530	CG	LEU	A1202	-28.179	8.895	12.287	1.00	51.46	A
1531	CD1	LEU	A1202	-29.495	9.423	12.228	1.00	56.71	A
1532	CD2	LEU	A1202	-28.310	7.474	11.874	1.00	53.16	A
1533	C	LEU	A1202	-26.380	11.277	9.687	1.00	51.88	A
1534	O	LEU	A1202	-26.938	11.070	8.649	1.00	47.85	A
1535	N	VAL	A1203	-25.047	11.193	9.767	1.00	51.85	A
1536	CA	VAL	A1203	-24.118	11.821	8.851	1.00	51.80	A
1537	CB	VAL	A1203	-24.084	13.332	9.156	1.00	52.63	A
1538	CG1	VAL	A1203	-25.488	13.958	8.937	1.00	52.65	A
1539	CG2	VAL	A1203	-23.515	13.612	10.681	1.00	52.59	A
1540	C	VAL	A1203	-22.732	11.374	9.186	1.00	51.71	A
1541	O	VAL	A1203	-22.408	11.269	10.363	1.00	50.79	A
1542	N	ALA	A1204	-21.901	11.197	8.144	1.00	52.43	A
1543	CA	ALA	A1204	-20.469	10.833	8.255	1.00	50.94	A
1544	CB	ALA	A1204	-19.645	11.141	6.963	1.00	51.03	A
1545	C	ALA	A1204	-19.971	11.634	9.395	1.00	51.08	A
1546	O	ALA	A1204	-20.803	12.117	10.196	1.00	49.64	A
1547	N	ARG	A1205	-18.648	11.618	9.560	1.00	51.32	A
1548	CA	ARG	A1205	-17.866	12.600	10.340	1.00	52.19	A
1549	CB	ARG	A1205	-16.604	12.890	9.460	1.00	52.76	A
1550	CG	ARG	A1205	-16.517	14.297	9.120	1.00	55.54	A
1551	CD	ARG	A1205	-17.431	14.648	7.859	1.00	57.71	A
1552	NE	ARG	A1205	-18.819	14.224	7.980	1.00	49.34	A
1553	CZ	ARG	A1205	-19.852	15.066	7.968	1.00	53.83	A
1554	NH1	ARG	A1205	-19.701	16.437	7.859	1.00	47.61	A
1555	NH2	ARG	A1205	-21.072	14.537	8.092	1.00	55.52	A

1556	C	ARG	A1205	-18.481	13.882	11.138	1.00	52.50	A
1557	O	ARG	A1205	-19.630	14.391	10.882	1.00	51.49	A
1558	N	PRO	A1206	-17.773	14.347	12.215	1.00	52.91	A
1559	CD	PRO	A1206	-16.572	13.895	12.947	1.00	55.09	A
1560	CA	PRO	A1206	-18.437	15.307	13.030	1.00	52.48	A
1561	CB	PRO	A1206	-18.163	14.787	14.470	1.00	50.04	A
1562	CG	PRO	A1206	-17.082	13.835	14.372	1.00	52.32	A
1563	C	PRO	A1206	-18.037	16.711	12.784	1.00	53.73	A
1564	O	PRO	A1206	-17.111	16.929	12.102	1.00	53.86	A
1565	N	GLU	A1207	-18.749	17.669	13.404	1.00	56.67	A
1566	CA	GLU	A1207	-18.880	19.077	12.955	1.00	57.30	A
1567	CB	GLU	A1207	-19.822	19.157	11.731	1.00	58.19	A
1568	CG	GLU	A1207	-21.327	18.841	12.005	1.00	56.23	A
1569	CD	GLU	A1207	-22.326	19.766	11.111	1.00	61.67	A
1570	OE1	GLU	A1207	-23.538	19.360	10.991	1.00	61.69	A
1571	OE2	GLU	A1207	-21.947	20.883	10.583	1.00	59.85	A
1572	C	GLU	A1207	-19.552	19.812	14.093	1.00	57.31	A
1573	O	GLU	A1207	-19.663	19.322	15.252	1.00	57.20	A
1574	N	PRO	A1208	-20.096	20.977	13.796	1.00	57.36	A
1575	CD	PRO	A1208	-20.662	21.741	12.645	1.00	57.99	A
1576	CA	PRO	A1208	-20.270	21.719	15.028	1.00	56.95	A
1577	CB	PRO	A1208	-20.819	23.079	14.493	1.00	57.92	A
1578	CG	PRO	A1208	-21.733	22.659	13.310	1.00	53.46	A
1579	C	PRO	A1208	-21.493	21.212	15.659	1.00	56.31	A
1580	O	PRO	A1208	-22.054	21.935	16.497	1.00	56.89	A
1581	N	ALA	A1209	-22.060	20.157	15.103	1.00	54.11	A
1582	CA	ALA	A1209	-23.453	20.008	15.369	1.00	53.49	A
1583	CB	ALA	A1209	-24.357	20.731	14.283	1.00	49.29	A
1584	C	ALA	A1209	-23.779	18.573	15.760	1.00	51.75	A
1585	O	ALA	A1209	-24.911	18.204	16.118	1.00	53.10	A
1586	N	THR	A1210	-22.739	17.813	15.858	1.00	49.97	A
1587	CA	THR	A1210	-22.914	16.486	16.357	1.00	52.14	A
1588	CB	THR	A1210	-22.094	15.481	15.503	1.00	50.07	A
1589	OG1	THR	A1210	-20.835	16.066	15.224	1.00	56.16	A
1590	CG2	THR	A1210	-22.618	15.278	14.201	1.00	42.68	A
1591	C	THR	A1210	-22.566	16.566	17.912	1.00	53.85	A
1592	O	THR	A1210	-23.134	15.860	18.707	1.00	55.38	A
1593	N	GLY	A1211	-21.681	17.459	18.354	1.00	54.89	A
1594	CA	GLY	A1211	-21.404	17.683	19.804	1.00	54.81	A
1595	C	GLY	A1211	-22.452	18.110	20.851	1.00	55.21	A
1596	O	GLY	A1211	-22.690	19.222	20.947	1.00	59.65	A
1597	N	TYR	A1212	-23.056	17.225	21.627	1.00	54.74	A
1598	CA	TYR	A1212	-24.015	17.410	22.764	1.00	52.12	A
1599	CB	TYR	A1212	-24.901	16.152	22.852	1.00	50.84	A
1600	CG	TYR	A1212	-25.707	15.987	21.534	1.00	47.51	A
1601	CD1	TYR	A1212	-27.035	16.325	21.468	1.00	45.57	A
1602	CE1	TYR	A1212	-27.764	16.298	20.280	1.00	48.73	A
1603	CD2	TYR	A1212	-25.157	15.454	20.416	1.00	48.94	A
1604	CE2	TYR	A1212	-25.919	15.319	19.188	1.00	46.71	A
1605	CZ	TYR	A1212	-27.166	15.854	19.138	1.00	45.21	A
1606	OH	TYR	A1212	-27.915	15.710	18.082	1.00	44.50	A
1607	C	TYR	A1212	-23.126	17.408	23.971	1.00	50.81	A
1608	O	TYR	A1212	-21.983	16.861	23.870	1.00	51.41	A
1609	N	THR	A1213	-23.487	18.137	25.022	1.00	48.87	A
1610	CA	THR	A1213	-22.679	18.065	26.310	1.00	47.53	A
1611	CB	THR	A1213	-22.625	19.369	26.957	1.00	46.92	A

1612	OG1	THR	A1213	-23.964	19.815	26.910	1.00	45.96	A
1613	CG2	THR	A1213	-21.770	20.460	26.116	1.00	49.78	A
1614	C	THR	A1213	-23.682	17.283	27.184	1.00	46.37	A
1615	O	THR	A1213	-24.877	17.668	27.093	1.00	43.28	A
1616	N	LEU	A1214	-23.323	16.173	27.893	1.00	45.11	A
1617	CA	LEU	A1214	-24.422	15.410	28.472	1.00	47.58	A
1618	CB	LEU	A1214	-24.060	13.972	28.980	1.00	47.46	A
1619	CG	LEU	A1214	-23.257	13.367	27.837	1.00	47.30	A
1620	CD1	LEU	A1214	-22.625	11.998	28.171	1.00	46.55	A
1621	CD2	LEU	A1214	-24.073	13.366	26.521	1.00	36.33	A
1622	C	LEU	A1214	-24.853	16.249	29.581	1.00	48.16	A
1623	O	LEU	A1214	-24.097	16.935	30.160	1.00	49.60	A
1624	N	GLU	A1215	-26.078	16.198	29.941	1.00	50.93	A
1625	CA	GLU	A1215	-26.386	16.767	31.236	1.00	53.09	A
1626	CB	GLU	A1215	-27.185	18.050	31.056	1.00	53.78	A
1627	CG	GLU	A1215	-27.118	19.040	32.391	1.00	55.21	A
1628	CD	GLU	A1215	-27.717	20.421	32.100	1.00	54.06	A
1629	OE1	GLU	A1215	-26.962	21.324	31.670	1.00	48.79	A
1630	OE2	GLU	A1215	-28.989	20.505	32.131	1.00	54.62	A
1631	C	GLU	A1215	-27.069	15.835	32.274	1.00	51.25	A
1632	O	GLU	A1215	-28.236	15.628	32.215	1.00	53.62	A
1633	N	PHE	A1216	-26.345	15.299	33.222	1.00	49.48	A
1634	CA	PHE	A1216	-26.945	14.350	34.164	1.00	50.28	A
1635	CB	PHE	A1216	-25.810	13.593	34.828	1.00	51.32	A
1636	CG	PHE	A1216	-24.879	12.932	33.818	1.00	44.77	A
1637	CD1	PHE	A1216	-25.304	11.925	33.080	1.00	39.43	A
1638	CD2	PHE	A1216	-23.717	13.434	33.552	1.00	38.47	A
1639	CE1	PHE	A1216	-24.535	11.270	32.226	1.00	40.89	A
1640	CE2	PHE	A1216	-22.973	12.829	32.595	1.00	47.64	A
1641	CZ	PHE	A1216	-23.417	11.677	31.937	1.00	44.22	A
1642	C	PHE	A1216	-27.925	14.915	35.208	1.00	51.91	A
1643	O	PHE	A1216	-27.839	16.106	35.541	1.00	51.72	A
1644	N	ARG	A1217	-28.937	14.092	35.557	1.00	51.98	A
1645	CA	ARG	A1217	-29.971	14.333	36.585	1.00	53.35	A
1646	CB	ARG	A1217	-31.237	14.945	36.034	1.00	51.43	A
1647	CG	ARG	A1217	-30.889	16.150	35.444	1.00	54.21	A
1648	CD	ARG	A1217	-31.960	17.081	35.339	1.00	60.03	A
1649	NE	ARG	A1217	-31.302	18.289	34.866	1.00	61.93	A
1650	CZ	ARG	A1217	-31.645	19.511	35.201	1.00	61.49	A
1651	NH1	ARG	A1217	-32.685	19.696	36.019	1.00	58.97	A
1652	NH2	ARG	A1217	-30.956	20.538	34.687	1.00	62.07	A
1653	C	ARG	A1217	-30.383	13.014	37.154	1.00	56.64	A
1654	O	ARG	A1217	-31.225	12.298	36.548	1.00	57.70	A
1655	N	SER	A1218	-29.773	12.681	38.304	1.00	58.24	A
1656	CA	SER	A1218	-29.926	11.348	39.039	1.00	56.57	A
1657	CB	SER	A1218	-30.752	11.666	40.306	1.00	55.69	A
1658	OG	SER	A1218	-31.816	12.506	39.736	1.00	51.77	A
1659	C	SER	A1218	-30.724	10.360	38.149	1.00	55.12	A
1660	O	SER	A1218	-31.878	10.612	37.940	1.00	56.40	A
1661	N	GLY	A1219	-30.121	9.296	37.624	1.00	53.88	A
1662	CA	GLY	A1219	-30.776	8.210	36.790	1.00	52.47	A
1663	C	GLY	A1219	-30.622	8.628	35.374	1.00	52.43	A
1664	O	GLY	A1219	-30.164	7.889	34.514	1.00	51.68	A
1665	N	LYS	A1220	-30.886	9.904	35.162	1.00	52.46	A
1666	CA	LYS	A1220	-31.091	10.375	33.914	1.00	52.88	A
1667	CB	LYS	A1220	-32.363	11.036	33.961	1.00	53.57	A

1668	CG	LYS	A1220	-33.269	10.254	34.912	1.00	47.05	A
1669	CD	LYS	A1220	-34.404	9.638	34.171	1.00	55.99	A
1670	CE	LYS	A1220	-34.097	8.097	34.168	1.00	56.35	A
1671	NZ	LYS	A1220	-34.452	7.630	35.532	1.00	44.34	A
1672	C	LYS	A1220	-30.055	11.302	33.422	1.00	56.04	A
1673	O	LYS	A1220	-29.263	11.903	34.295	1.00	57.59	A
1674	N	VAL	A1221	-30.049	11.412	32.048	1.00	54.93	A
1675	CA	VAL	A1221	-29.161	12.348	31.315	1.00	54.81	A
1676	CB	VAL	A1221	-27.977	11.581	30.743	1.00	53.65	A
1677	CG1	VAL	A1221	-28.445	10.685	29.696	1.00	55.71	A
1678	CG2	VAL	A1221	-26.945	12.424	30.174	1.00	53.99	A
1679	C	VAL	A1221	-30.000	13.019	30.237	1.00	54.84	A
1680	O	VAL	A1221	-31.044	12.458	29.739	1.00	55.57	A
1681	N	ALA	A1222	-29.535	14.188	29.857	1.00	53.40	A
1682	CA	ALA	A1222	-30.201	14.972	28.807	1.00	53.03	A
1683	CB	ALA	A1222	-31.095	15.978	29.411	1.00	52.24	A
1684	C	ALA	A1222	-29.128	15.653	27.874	1.00	53.61	A
1685	O	ALA	A1222	-27.847	15.720	28.166	1.00	51.21	A
1686	N	PHE	A1223	-29.572	16.126	26.699	1.00	52.35	A
1687	CA	PHE	A1223	-28.453	16.475	25.801	1.00	52.12	A
1688	CB	PHE	A1223	-28.369	15.436	24.698	1.00	48.73	A
1689	CG	PHE	A1223	-28.331	14.009	25.158	1.00	49.43	A
1690	CD1	PHE	A1223	-27.119	13.413	25.578	1.00	49.37	A
1691	CD2	PHE	A1223	-29.436	13.171	24.885	1.00	51.43	A
1692	CE1	PHE	A1223	-26.963	12.053	25.739	1.00	42.48	A
1693	CE2	PHE	A1223	-29.331	11.813	25.010	1.00	49.72	A
1694	CZ	PHE	A1223	-28.017	11.244	25.477	1.00	52.67	A
1695	C	PHE	A1223	-28.414	17.823	25.132	1.00	51.66	A
1696	O	PHE	A1223	-29.377	18.148	24.380	1.00	49.85	A
1697	N	ARG	A1224	-27.278	18.543	25.239	1.00	51.48	A
1698	CA	ARG	A1224	-27.383	19.908	24.713	1.00	52.69	A
1699	CB	ARG	A1224	-27.162	21.059	25.678	1.00	50.65	A
1700	CG	ARG	A1224	-25.876	21.627	25.478	1.00	48.65	A
1701	CD	ARG	A1224	-25.529	23.029	26.240	1.00	53.91	A
1702	NE	ARG	A1224	-26.479	23.203	27.337	1.00	60.13	A
1703	CZ	ARG	A1224	-26.928	24.344	27.845	1.00	53.57	A
1704	NH1	ARG	A1224	-26.517	25.547	27.335	1.00	51.86	A
1705	NH2	ARG	A1224	-27.827	24.208	28.833	1.00	45.78	A
1706	C	ARG	A1224	-26.449	20.125	23.730	1.00	56.06	A
1707	O	ARG	A1224	-25.191	20.166	24.025	1.00	57.79	A
1708	N	ASP	A1225	-27.066	20.351	22.552	1.00	59.47	A
1709	CA	ASP	A1225	-26.386	20.698	21.334	1.00	61.55	A
1710	CB	ASP	A1225	-27.380	20.797	20.238	1.00	60.84	A
1711	CG	ASP	A1225	-27.774	22.252	19.950	1.00	61.50	A
1712	OD1	ASP	A1225	-26.910	23.176	19.861	1.00	49.06	A
1713	OD2	ASP	A1225	-28.995	22.465	19.746	1.00	65.92	A
1714	C	ASP	A1225	-25.707	22.091	21.525	1.00	64.13	A
1715	O	ASP	A1225	-26.062	22.810	22.510	1.00	66.64	A
1716	N	CYS	A1226	-24.784	22.453	20.577	1.00	63.90	A
1717	CA	CYS	A1226	-23.990	23.690	20.475	1.00	62.63	A
1718	CB	CYS	A1226	-23.120	23.600	19.202	1.00	63.70	A
1719	SG	CYS	A1226	-24.122	23.317	17.556	1.00	57.17	A
1720	C	CYS	A1226	-24.792	25.019	20.380	1.00	64.24	A
1721	O	CYS	A1226	-24.242	26.093	20.008	1.00	66.01	A
1722	N	GLU	A1227	-26.087	24.954	20.583	1.00	62.70	A
1723	CA	GLU	A1227	-26.879	26.150	20.470	1.00	63.51	A

1724	CB	GLU	A1227	-27.978	26.040	19.316	1.00	63.57	A
1725	CG	GLU	A1227	-27.673	26.251	17.740	1.00	59.82	A
1726	CD	GLU	A1227	-26.399	27.039	17.195	1.00	63.84	A
1727	OE1	GLU	A1227	-26.159	28.300	17.415	1.00	66.16	A
1728	OE2	GLU	A1227	-25.682	26.390	16.377	1.00	56.40	A
1729	C	GLU	A1227	-27.511	26.442	21.914	1.00	64.20	A
1730	O	GLU	A1227	-27.341	27.561	22.455	1.00	65.41	A
1731	N	GLY	A1228	-28.217	25.437	22.479	1.00	61.97	A
1732	CA	GLY	A1228	-28.691	25.361	23.838	1.00	59.70	A
1733	C	GLY	A1228	-30.035	24.672	23.702	1.00	57.81	A
1734	O	GLY	A1228	-31.014	25.110	24.183	1.00	58.22	A
1735	N	ARG	A1229	-30.128	23.535	23.093	1.00	57.52	A
1736	CA	ARG	A1229	-31.410	23.198	22.611	1.00	58.85	A
1737	CB	ARG	A1229	-31.511	23.511	21.087	1.00	58.72	A
1738	CG	ARG	A1229	-30.657	24.657	20.382	1.00	57.38	A
1739	CD	ARG	A1229	-31.085	24.645	18.817	1.00	62.21	A
1740	NE	ARG	A1229	-30.826	23.370	18.065	1.00	77.52	A
1741	CZ	ARG	A1229	-31.666	22.731	17.183	1.00	79.23	A
1742	NH1	ARG	A1229	-32.919	23.205	16.915	1.00	80.63	A
1743	NH2	ARG	A1229	-31.267	21.593	16.560	1.00	71.78	A
1744	C	ARG	A1229	-31.585	21.731	22.761	1.00	60.80	A
1745	O	ARG	A1229	-31.846	21.012	21.724	1.00	58.38	A
1746	N	TYR	A1230	-31.352	21.278	24.016	1.00	62.14	A
1747	CA	TYR	A1230	-31.724	19.926	24.498	1.00	63.40	A
1748	CB	TYR	A1230	-32.505	19.984	25.791	1.00	64.04	A
1749	CG	TYR	A1230	-31.560	20.508	26.886	1.00	68.93	A
1750	CD1	TYR	A1230	-31.649	21.849	27.351	1.00	60.29	A
1751	CE1	TYR	A1230	-30.706	22.319	28.340	1.00	70.46	A
1752	CD2	TYR	A1230	-30.486	19.643	27.426	1.00	71.05	A
1753	CE2	TYR	A1230	-29.515	20.110	28.438	1.00	67.36	A
1754	CZ	TYR	A1230	-29.657	21.448	28.963	1.00	70.91	A
1755	OH	TYR	A1230	-28.779	21.980	30.010	1.00	64.46	A
1756	C	TYR	A1230	-32.314	18.885	23.556	1.00	62.43	A
1757	O	TYR	A1230	-33.344	19.085	23.002	1.00	60.96	A
1758	N	LEU	A1231	-31.604	17.765	23.393	1.00	62.11	A
1759	CA	LEU	A1231	-32.144	16.680	22.597	1.00	62.94	A
1760	CB	LEU	A1231	-31.138	15.474	22.496	1.00	62.84	A
1761	CG	LEU	A1231	-30.967	14.839	21.011	1.00	68.34	A
1762	CD1	LEU	A1231	-31.049	15.722	19.668	1.00	49.27	A
1763	CD2	LEU	A1231	-29.621	14.058	20.866	1.00	64.93	A
1764	C	LEU	A1231	-33.637	16.268	22.952	1.00	60.44	A
1765	O	LEU	A1231	-34.103	16.445	24.110	1.00	60.78	A
1766	N	ALA	A1232	-34.376	15.787	21.965	1.00	56.47	A
1767	CA	ALA	A1232	-35.549	15.075	22.299	1.00	56.66	A
1768	CB	ALA	A1232	-36.396	15.853	23.326	1.00	58.67	A
1769	C	ALA	A1232	-36.392	14.584	21.150	1.00	56.19	A
1770	O	ALA	A1232	-36.322	15.235	20.104	1.00	54.58	A
1771	N	PRO	A1233	-37.202	13.469	21.368	1.00	55.23	A
1772	CD	PRO	A1233	-37.341	12.737	22.616	1.00	53.53	A
1773	CA	PRO	A1233	-38.094	12.859	20.383	1.00	58.42	A
1774	CB	PRO	A1233	-38.918	11.848	21.228	1.00	56.20	A
1775	CG	PRO	A1233	-38.033	11.492	22.230	1.00	52.89	A
1776	C	PRO	A1233	-38.966	13.875	19.482	1.00	59.90	A
1777	O	PRO	A1233	-38.665	15.075	19.450	1.00	59.94	A
1778	N	SER	A1234	-39.973	13.399	18.726	1.00	61.92	A
1779	CA	SER	A1234	-40.745	14.261	17.764	1.00	62.11	A

1780	CB	SER	A1234	-39.910	14.680	16.570	1.00	62.78	A
1781	OG	SER	A1234	-38.591	15.052	17.020	1.00	59.06	A
1782	C	SER	A1234	-42.019	13.671	17.312	1.00	62.46	A
1783	O	SER	A1234	-43.014	13.918	17.899	1.00	65.41	A
1784	N	GLY	A1235	-42.044	12.882	16.286	1.00	63.33	A
1785	CA	GLY	A1235	-43.364	12.283	15.966	1.00	64.32	A
1786	C	GLY	A1235	-43.694	11.018	16.759	1.00	63.69	A
1787	O	GLY	A1235	-43.210	10.817	17.916	1.00	63.28	A
1788	N	PRO	A1236	-44.470	10.151	16.121	1.00	64.01	A
1789	CD	PRO	A1236	-45.135	10.673	14.917	1.00	65.58	A
1790	CA	PRO	A1236	-44.842	8.736	16.373	1.00	65.05	A
1791	CB	PRO	A1236	-45.902	8.402	15.264	1.00	64.27	A
1792	CG	PRO	A1236	-45.534	9.403	14.139	1.00	68.08	A
1793	C	PRO	A1236	-43.622	7.856	16.183	1.00	62.98	A
1794	O	PRO	A1236	-43.656	6.633	16.448	1.00	63.68	A
1795	N	SER	A1237	-42.578	8.505	15.744	1.00	61.00	A
1796	CA	SER	A1237	-41.290	7.869	15.651	1.00	62.60	A
1797	CB	SER	A1237	-40.895	7.865	14.163	1.00	64.27	A
1798	OG	SER	A1237	-40.943	9.237	13.597	1.00	64.10	A
1799	C	SER	A1237	-40.237	8.694	16.508	1.00	61.96	A
1800	O	SER	A1237	-39.243	9.190	15.990	1.00	61.05	A
1801	N	GLY	A1238	-40.554	8.921	17.784	1.00	60.38	A
1802	CA	GLY	A1238	-39.671	9.513	18.720	1.00	57.37	A
1803	C	GLY	A1238	-38.510	10.149	17.985	1.00	56.67	A
1804	O	GLY	A1238	-37.451	10.299	18.619	1.00	54.97	A
1805	N	THR	A1239	-38.706	10.582	16.706	1.00	52.71	A
1806	CA	THR	A1239	-37.504	10.984	15.888	1.00	51.87	A
1807	CB	THR	A1239	-37.858	11.736	14.581	1.00	48.97	A
1808	OG1	THR	A1239	-38.327	10.730	13.687	1.00	58.00	A
1809	CG2	THR	A1239	-36.741	12.376	13.931	1.00	43.00	A
1810	C	THR	A1239	-36.611	11.690	16.786	1.00	52.07	A
1811	O	THR	A1239	-37.025	12.674	17.387	1.00	54.36	A
1812	N	LEU	A1240	-35.409	11.193	16.937	1.00	53.28	A
1813	CA	LEU	A1240	-34.529	11.753	17.950	1.00	55.51	A
1814	CB	LEU	A1240	-33.539	10.706	18.581	1.00	54.14	A
1815	CG	LEU	A1240	-33.452	10.719	20.169	1.00	56.36	A
1816	CD1	LEU	A1240	-32.245	10.007	20.773	1.00	47.97	A
1817	CD2	LEU	A1240	-33.507	12.159	20.957	1.00	49.51	A
1818	C	LEU	A1240	-33.852	13.029	17.453	1.00	56.46	A
1819	O	LEU	A1240	-32.945	12.943	16.765	1.00	59.82	A
1820	N	LYS	A1241	-34.324	14.220	17.790	1.00	57.68	A
1821	CA	LYS	A1241	-33.699	15.432	17.313	1.00	58.06	A
1822	CB	LYS	A1241	-34.521	15.829	16.124	1.00	59.73	A
1823	CG	LYS	A1241	-36.042	15.557	16.392	1.00	58.68	A
1824	CD	LYS	A1241	-36.744	15.539	15.078	1.00	57.25	A
1825	CE	LYS	A1241	-37.465	16.766	14.782	1.00	53.04	A
1826	NZ	LYS	A1241	-38.806	16.209	15.102	1.00	57.12	A
1827	C	LYS	A1241	-33.760	16.622	18.295	1.00	58.42	A
1828	O	LYS	A1241	-34.829	16.904	18.813	1.00	57.40	A
1829	N	ALA	A1242	-32.651	17.338	18.519	1.00	58.72	A
1830	CA	ALA	A1242	-32.700	18.611	19.274	1.00	58.71	A
1831	CB	ALA	A1242	-31.877	19.664	18.641	1.00	59.35	A
1832	C	ALA	A1242	-34.071	19.163	19.476	1.00	58.72	A
1833	O	ALA	A1242	-35.061	18.513	19.144	1.00	58.95	A
1834	N	GLY	A1243	-34.121	20.370	20.029	1.00	59.24	A
1835	CA	GLY	A1243	-35.390	20.940	20.550	1.00	62.05	A

1836	C	GLY	A1243	-35.230	22.391	20.988	1.00	62.71	A
1837	O	GLY	A1243	-34.161	22.914	21.028	1.00	61.95	A
1838	N	LYS	A1244	-36.310	23.031	21.362	1.00	64.53	A
1839	CA	LYS	A1244	-36.258	24.499	21.557	1.00	64.63	A
1840	CB	LYS	A1244	-37.358	25.185	20.662	1.00	63.49	A
1841	CG	LYS	A1244	-38.689	24.577	20.647	1.00	53.76	A
1842	CD	LYS	A1244	-38.904	23.772	19.420	1.00	54.27	A
1843	CE	LYS	A1244	-38.949	24.585	18.162	1.00	53.37	A
1844	NZ	LYS	A1244	-37.676	25.383	17.661	1.00	58.03	A
1845	C	LYS	A1244	-36.517	24.872	23.040	1.00	65.49	A
1846	O	LYS	A1244	-36.531	26.035	23.357	1.00	65.75	A
1847	N	ALA	A1245	-36.782	23.870	23.897	1.00	65.90	A
1848	CA	ALA	A1245	-37.144	24.015	25.293	1.00	63.80	A
1849	CB	ALA	A1245	-37.487	22.643	25.817	1.00	64.64	A
1850	C	ALA	A1245	-35.977	24.605	26.034	1.00	63.72	A
1851	O	ALA	A1245	-34.834	24.131	25.856	1.00	59.78	A
1852	N	THR	A1246	-36.277	25.710	26.793	1.00	65.16	A
1853	CA	THR	A1246	-35.294	26.440	27.694	1.00	63.05	A
1854	CB	THR	A1246	-35.988	27.671	28.557	1.00	64.23	A
1855	OG1	THR	A1246	-37.230	27.288	29.180	1.00	64.17	A
1856	CG2	THR	A1246	-36.225	29.167	27.837	1.00	58.43	A
1857	C	THR	A1246	-34.447	25.370	28.600	1.00	63.72	A
1858	O	THR	A1246	-33.210	25.057	28.348	1.00	63.78	A
1859	N	LYS	A1247	-35.098	24.762	29.594	1.00	63.32	A
1860	CA	LYS	A1247	-34.387	23.892	30.597	1.00	63.10	A
1861	CB	LYS	A1247	-34.435	24.517	32.077	1.00	63.59	A
1862	CG	LYS	A1247	-34.078	26.011	32.364	1.00	62.45	A
1863	CD	LYS	A1247	-34.834	26.588	33.605	1.00	61.45	A
1864	CE	LYS	A1247	-34.143	27.926	34.330	1.00	65.20	A
1865	NZ	LYS	A1247	-34.593	28.690	35.811	1.00	58.00	A
1866	C	LYS	A1247	-35.194	22.545	30.668	1.00	62.81	A
1867	O	LYS	A1247	-36.434	22.602	30.831	1.00	63.10	A
1868	N	VAL	A1248	-34.493	21.408	30.725	1.00	61.20	A
1869	CA	VAL	A1248	-34.952	20.079	30.459	1.00	60.29	A
1870	CB	VAL	A1248	-33.747	19.025	30.724	1.00	61.88	A
1871	CG1	VAL	A1248	-33.459	18.585	32.230	1.00	64.28	A
1872	CG2	VAL	A1248	-33.720	17.707	29.743	1.00	65.29	A
1873	C	VAL	A1248	-36.255	19.862	31.165	1.00	60.53	A
1874	O	VAL	A1248	-36.726	20.796	31.900	1.00	61.32	A
1875	N	GLY	A1249	-36.895	18.691	30.957	1.00	58.00	A
1876	CA	GLY	A1249	-38.144	18.417	31.669	1.00	54.79	A
1877	C	GLY	A1249	-38.186	16.975	31.499	1.00	55.25	A
1878	O	GLY	A1249	-37.103	16.460	31.164	1.00	55.94	A
1879	N	LYS	A1250	-39.372	16.337	31.670	1.00	56.52	A
1880	CA	LYS	A1250	-39.627	14.857	31.451	1.00	58.35	A
1881	CB	LYS	A1250	-41.018	14.361	31.847	1.00	60.21	A
1882	CG	LYS	A1250	-42.211	14.946	31.038	1.00	57.62	A
1883	CD	LYS	A1250	-43.590	14.589	31.745	1.00	54.39	A
1884	CE	LYS	A1250	-43.973	15.513	32.923	1.00	45.38	A
1885	NZ	LYS	A1250	-43.579	16.997	32.959	1.00	47.32	A
1886	C	LYS	A1250	-39.468	14.356	30.038	1.00	61.04	A
1887	O	LYS	A1250	-38.532	13.615	29.818	1.00	65.55	A
1888	N	ASP	A1251	-40.421	14.623	29.121	1.00	60.46	A
1889	CA	ASP	A1251	-40.084	14.843	27.709	1.00	58.35	A
1890	CB	ASP	A1251	-40.270	16.301	27.280	1.00	60.51	A
1891	CG	ASP	A1251	-40.210	17.326	28.567	1.00	64.08	A

1892	OD1	ASP	A1251	-41.297	17.809	29.088	1.00	61.40	A
1893	OD2	ASP	A1251	-39.079	17.516	29.075	1.00	59.92	A
1894	C	ASP	A1251	-38.657	14.492	27.418	1.00	56.03	A
1895	O	ASP	A1251	-38.437	13.482	26.604	1.00	55.36	A
1896	N	GLU	A1252	-37.705	15.227	28.029	1.00	50.40	A
1897	CA	GLU	A1252	-36.271	15.094	27.466	1.00	49.71	A
1898	CB	GLU	A1252	-35.586	16.437	27.295	1.00	47.66	A
1899	CG	GLU	A1252	-36.590	17.486	27.562	1.00	49.20	A
1900	CD	GLU	A1252	-36.045	18.725	27.334	1.00	42.01	A
1901	OE1	GLU	A1252	-36.728	19.857	27.404	1.00	46.11	A
1902	OE2	GLU	A1252	-34.862	18.508	27.121	1.00	39.77	A
1903	C	GLU	A1252	-35.274	14.206	28.224	1.00	49.28	A
1904	O	GLU	A1252	-34.032	14.388	28.167	1.00	48.41	A
1905	N	LEU	A1253	-35.820	13.256	28.940	1.00	49.59	A
1906	CA	LEU	A1253	-34.971	12.561	29.872	1.00	51.69	A
1907	CB	LEU	A1253	-35.545	12.495	31.381	1.00	52.95	A
1908	CG	LEU	A1253	-35.456	13.932	32.045	1.00	53.96	A
1909	CD1	LEU	A1253	-35.475	13.943	33.599	1.00	52.42	A
1910	CD2	LEU	A1253	-34.356	14.786	31.661	1.00	48.25	A
1911	C	LEU	A1253	-34.778	11.197	29.303	1.00	50.64	A
1912	O	LEU	A1253	-35.848	10.559	29.010	1.00	50.38	A
1913	N	PHE	A1254	-33.472	10.833	29.127	1.00	47.18	A
1914	CA	PHE	A1254	-33.082	9.524	28.929	1.00	46.70	A
1915	CB	PHE	A1254	-32.362	9.330	27.569	1.00	45.57	A
1916	CG	PHE	A1254	-32.813	10.263	26.572	1.00	45.71	A
1917	CD1	PHE	A1254	-33.885	10.001	25.873	1.00	40.21	A
1918	CD2	PHE	A1254	-32.133	11.479	26.354	1.00	45.22	A
1919	CE1	PHE	A1254	-34.380	11.027	25.009	1.00	48.57	A
1920	CE2	PHE	A1254	-32.638	12.459	25.596	1.00	43.99	A
1921	CZ	PHE	A1254	-33.796	12.222	24.897	1.00	43.85	A
1922	C	PHE	A1254	-32.351	8.814	30.097	1.00	48.18	A
1923	O	PHE	A1254	-31.446	9.385	30.716	1.00	48.46	A
1924	N	ALA	A1255	-32.671	7.521	30.258	1.00	48.73	A
1925	CA	ALA	A1255	-31.897	6.627	30.984	1.00	49.88	A
1926	CB	ALA	A1255	-32.767	5.770	31.862	1.00	49.04	A
1927	C	ALA	A1255	-31.077	5.715	30.042	1.00	51.35	A
1928	O	ALA	A1255	-31.669	4.966	29.372	1.00	55.33	A
1929	N	LEU	A1256	-29.725	5.673	30.108	1.00	50.85	A
1930	CA	LEU	A1256	-28.909	4.869	29.264	1.00	48.78	A
1931	CB	LEU	A1256	-27.585	5.642	28.920	1.00	49.57	A
1932	CG	LEU	A1256	-27.624	7.174	28.528	1.00	47.97	A
1933	CD1	LEU	A1256	-26.270	7.965	28.454	1.00	45.30	A
1934	CD2	LEU	A1256	-28.688	7.770	27.470	1.00	37.83	A
1935	C	LEU	A1256	-28.703	3.695	30.088	1.00	48.66	A
1936	O	LEU	A1256	-28.530	3.869	31.293	1.00	49.64	A
1937	N	GLU	A1257	-28.731	2.478	29.497	1.00	47.77	A
1938	CA	GLU	A1257	-28.631	1.223	30.321	1.00	47.36	A
1939	CB	GLU	A1257	-29.943	0.442	30.347	1.00	47.62	A
1940	CG	GLU	A1257	-31.167	1.167	29.661	1.00	49.14	A
1941	CD	GLU	A1257	-32.476	0.699	30.149	1.00	47.74	A
1942	OE1	GLU	A1257	-32.670	-0.465	29.961	1.00	49.70	A
1943	OE2	GLU	A1257	-33.339	1.432	30.702	1.00	46.47	A
1944	C	GLU	A1257	-27.488	0.309	29.875	1.00	49.43	A
1945	O	GLU	A1257	-26.884	0.525	28.841	1.00	53.65	A
1946	N	GLN	A1258	-27.108	-0.694	30.633	1.00	49.31	A
1947	CA	GLN	A1258	-25.981	-1.444	30.216	1.00	48.50	A

1948	CB	GLN	A1258	-25.522	-2.418	31.347	1.00	50.03	A
1949	CG	GLN	A1258	-24.485	-2.001	32.557	1.00	52.07	A
1950	CD	GLN	A1258	-23.838	-3.270	33.324	1.00	48.58	A
1951	OE1	GLN	A1258	-24.578	-4.238	33.681	1.00	50.22	A
1952	NE2	GLN	A1258	-22.514	-3.297	33.497	1.00	38.25	A
1953	C	GLN	A1258	-26.513	-2.247	28.980	1.00	49.22	A
1954	O	GLN	A1258	-27.483	-3.036	29.166	1.00	49.63	A
1955	N	SER	A1259	-25.896	-2.104	27.758	1.00	46.91	A
1956	CA	SER	A1259	-26.009	-3.126	26.712	1.00	44.38	A
1957	CB	SER	A1259	-25.301	-2.638	25.506	1.00	46.28	A
1958	OG	SER	A1259	-25.463	-3.426	24.306	1.00	47.23	A
1959	C	SER	A1259	-25.421	-4.463	26.960	1.00	45.72	A
1960	O	SER	A1259	-24.173	-4.575	26.899	1.00	50.32	A
1961	N	CYS	A1260	-26.213	-5.522	27.035	1.00	46.58	A
1962	CA	CYS	A1260	-25.731	-6.899	27.186	1.00	45.72	A
1963	CB	CYS	A1260	-26.799	-7.664	27.942	1.00	49.84	A
1964	SG	CYS	A1260	-26.448	-9.330	28.719	1.00	52.29	A
1965	C	CYS	A1260	-25.540	-7.551	25.828	1.00	46.16	A
1966	O	CYS	A1260	-26.107	-7.094	24.853	1.00	45.33	A
1967	N	ALA	A1261	-24.705	-8.587	25.769	1.00	45.39	A
1968	CA	ALA	A1261	-24.237	-9.096	24.517	1.00	47.61	A
1969	CB	ALA	A1261	-22.994	-9.926	24.690	1.00	44.84	A
1970	C	ALA	A1261	-25.354	-9.896	23.873	1.00	49.18	A
1971	O	ALA	A1261	-25.855	-10.880	24.503	1.00	53.58	A
1972	N	GLN	A1262	-25.767	-9.541	22.660	1.00	47.00	A
1973	CA	GLN	A1262	-26.883	-10.265	22.114	1.00	46.65	A
1974	CB	GLN	A1262	-27.822	-9.283	21.475	1.00	49.30	A
1975	CG	GLN	A1262	-29.227	-9.358	21.784	1.00	50.78	A
1976	CD	GLN	A1262	-29.690	-8.436	22.926	1.00	52.76	A
1977	OE1	GLN	A1262	-29.530	-7.257	22.843	1.00	51.91	A
1978	NE2	GLN	A1262	-30.419	-8.979	23.905	1.00	56.16	A
1979	C	GLN	A1262	-26.257	-11.095	21.064	1.00	45.25	A
1980	O	GLN	A1262	-25.388	-10.695	20.351	1.00	43.29	A
1981	N	VAL	A1263	-26.732	-12.298	20.945	1.00	47.61	A
1982	CA	VAL	A1263	-26.071	-13.461	20.128	1.00	44.24	A
1983	CB	VAL	A1263	-25.605	-14.641	21.027	1.00	44.47	A
1984	CG1	VAL	A1263	-24.227	-14.701	21.109	1.00	47.46	A
1985	CG2	VAL	A1263	-26.291	-14.559	22.530	1.00	43.71	A
1986	C	VAL	A1263	-27.067	-14.247	19.290	1.00	42.49	A
1987	O	VAL	A1263	-28.261	-14.298	19.530	1.00	39.77	A
1988	N	VAL	A1264	-26.483	-14.901	18.343	1.00	44.10	A
1989	CA	VAL	A1264	-27.122	-15.748	17.416	1.00	44.97	A
1990	CB	VAL	A1264	-27.025	-15.104	16.053	1.00	47.14	A
1991	CG1	VAL	A1264	-26.757	-16.204	14.772	1.00	50.51	A
1992	CG2	VAL	A1264	-28.220	-14.085	15.788	1.00	42.27	A
1993	C	VAL	A1264	-26.262	-16.974	17.523	1.00	44.75	A
1994	O	VAL	A1264	-25.057	-16.930	17.463	1.00	44.44	A
1995	N	LEU	A1265	-26.943	-18.036	17.758	1.00	46.47	A
1996	CA	LEU	A1265	-26.483	-19.350	17.964	1.00	49.28	A
1997	CB	LEU	A1265	-27.338	-19.708	19.169	1.00	49.87	A
1998	CG	LEU	A1265	-26.719	-19.143	20.459	1.00	44.76	A
1999	CD1	LEU	A1265	-27.734	-18.925	21.484	1.00	33.99	A
2000	CD2	LEU	A1265	-25.795	-20.371	20.849	1.00	38.97	A
2001	C	LEU	A1265	-26.852	-20.294	16.771	1.00	51.57	A
2002	O	LEU	A1265	-28.075	-20.415	16.330	1.00	52.77	A
2003	N	GLN	A1266	-25.857	-20.965	16.218	1.00	49.83	A

2004	CA	GLN	A1266	-26.142	-21.723	14.916	1.00	50.84	A
2005	CB	GLN	A1266	-25.126	-21.470	13.709	1.00	51.55	A
2006	CG	GLN	A1266	-25.567	-21.776	12.224	1.00	43.04	A
2007	CD	GLN	A1266	-24.451	-21.298	11.244	1.00	43.42	A
2008	OE1	GLN	A1266	-23.478	-22.023	11.006	1.00	33.27	A
2009	NE2	GLN	A1266	-24.496	-20.082	10.817	1.00	31.22	A
2010	C	GLN	A1266	-25.931	-23.106	15.248	1.00	52.93	A
2011	O	GLN	A1266	-25.051	-23.405	16.174	1.00	52.88	A
2012	N	ALA	A1267	-26.578	-23.951	14.422	1.00	52.65	A
2013	CA	ALA	A1267	-26.540	-25.440	14.686	1.00	51.11	A
2014	CB	ALA	A1267	-27.813	-25.982	14.474	1.00	50.66	A
2015	C	ALA	A1267	-25.556	-26.050	13.822	1.00	49.58	A
2016	O	ALA	A1267	-24.943	-25.339	13.045	1.00	51.99	A
2017	N	ALA	A1268	-25.261	-27.308	13.999	1.00	50.87	A
2018	CA	ALA	A1268	-24.449	-28.021	13.007	1.00	51.53	A
2019	CB	ALA	A1268	-24.154	-29.313	13.388	1.00	49.16	A
2020	C	ALA	A1268	-25.123	-28.001	11.607	1.00	54.82	A
2021	O	ALA	A1268	-24.395	-27.764	10.579	1.00	57.07	A
2022	N	ASN	A1269	-26.466	-28.225	11.551	1.00	55.26	A
2023	CA	ASN	A1269	-27.306	-28.397	10.259	1.00	52.37	A
2024	CB	ASN	A1269	-28.804	-28.622	10.544	1.00	51.64	A
2025	CG	ASN	A1269	-29.289	-27.572	11.464	1.00	50.17	A
2026	OD1	ASN	A1269	-28.419	-26.834	11.845	1.00	59.58	A
2027	ND2	ASN	A1269	-30.548	-27.509	11.933	1.00	46.37	A
2028	C	ASN	A1269	-27.325	-27.009	9.706	1.00	54.22	A
2029	O	ASN	A1269	-28.475	-26.528	9.040	1.00	50.71	A
2030	N	GLU	A1270	-26.162	-26.357	10.060	1.00	51.83	A
2031	CA	GLU	A1270	-25.859	-24.997	9.653	1.00	54.53	A
2032	CB	GLU	A1270	-25.695	-24.941	8.116	1.00	57.05	A
2033	CG	GLU	A1270	-24.839	-26.041	7.497	1.00	62.14	A
2034	CD	GLU	A1270	-23.415	-25.807	7.928	1.00	73.47	A
2035	OE1	GLU	A1270	-22.607	-25.239	7.103	1.00	76.14	A
2036	OE2	GLU	A1270	-23.132	-26.155	9.124	1.00	77.02	A
2037	C	GLU	A1270	-27.009	-24.033	9.956	1.00	53.08	A
2038	O	GLU	A1270	-26.968	-22.933	9.596	1.00	54.60	A
2039	N	ARG	A1271	-28.083	-24.430	10.535	1.00	52.10	A
2040	CA	ARG	A1271	-29.111	-23.471	10.611	1.00	53.73	A
2041	CB	ARG	A1271	-30.612	-24.046	10.417	1.00	55.12	A
2042	CG	ARG	A1271	-31.073	-24.660	9.026	1.00	55.75	A
2043	CD	ARG	A1271	-30.740	-23.879	7.792	1.00	59.58	A
2044	NE	ARG	A1271	-31.770	-22.918	7.427	1.00	56.92	A
2045	CZ	ARG	A1271	-33.026	-23.276	7.426	1.00	55.62	A
2046	NH1	ARG	A1271	-33.277	-24.514	7.791	1.00	53.47	A
2047	NH2	ARG	A1271	-33.999	-22.395	7.135	1.00	56.51	A
2048	C	ARG	A1271	-28.968	-22.822	11.984	1.00	53.94	A
2049	O	ARG	A1271	-28.190	-23.263	12.857	1.00	53.73	A
2050	N	ASN	A1272	-29.797	-21.781	12.125	1.00	53.81	A
2051	CA	ASN	A1272	-30.001	-21.011	13.293	1.00	54.01	A
2052	CB	ASN	A1272	-30.014	-19.595	12.794	1.00	55.69	A
2053	CG	ASN	A1272	-28.644	-19.034	12.602	1.00	55.62	A
2054	OD1	ASN	A1272	-27.575	-19.741	12.551	1.00	62.85	A
2055	ND2	ASN	A1272	-28.644	-17.769	12.498	1.00	41.76	A
2056	C	ASN	A1272	-31.314	-21.103	13.900	1.00	53.33	A
2057	O	ASN	A1272	-32.332	-21.177	13.218	1.00	52.16	A
2058	N	VAL	A1273	-31.284	-20.784	15.175	1.00	54.43	A
2059	CA	VAL	A1273	-32.428	-21.025	16.080	1.00	54.62	A

2060	CB	VAL	A1273	-32.023	-21.811	17.407	1.00	52.55	A
2061	CG1	VAL	A1273	-30.618	-22.040	17.453	1.00	49.49	A
2062	CG2	VAL	A1273	-32.439	-21.160	18.592	1.00	50.07	A
2063	C	VAL	A1273	-33.353	-19.865	16.287	1.00	55.67	A
2064	O	VAL	A1273	-32.931	-18.741	16.544	1.00	59.47	A
2065	N	SER	A1274	-34.635	-20.160	16.266	1.00	55.14	A
2066	CA	SER	A1274	-35.661	-19.172	16.182	1.00	52.55	A
2067	CB	SER	A1274	-36.405	-19.248	14.815	1.00	52.54	A
2068	OG	SER	A1274	-36.965	-17.954	14.430	1.00	55.62	A
2069	C	SER	A1274	-36.609	-19.508	17.129	1.00	50.16	A
2070	O	SER	A1274	-36.705	-20.594	17.516	1.00	49.36	A
2071	N	GLY	A1275	-37.284	-18.481	17.547	1.00	53.13	A
2072	CA	GLY	A1275	-38.593	-18.494	18.195	1.00	53.02	A
2073	C	GLY	A1275	-39.628	-18.598	17.111	1.00	53.26	A
2074	O	GLY	A1275	-40.723	-18.902	17.426	1.00	52.63	A
2075	N	ARG	A1276	-39.217	-18.533	15.819	1.00	56.33	A
2076	CA	ARG	A1276	-40.124	-18.546	14.618	1.00	57.25	A
2077	CB	ARG	A1276	-39.427	-18.247	13.275	1.00	56.40	A
2078	CG	ARG	A1276	-39.843	-17.004	12.567	1.00	52.36	A
2079	CD	ARG	A1276	-38.692	-16.560	11.627	1.00	54.55	A
2080	NE	ARG	A1276	-38.479	-15.112	11.283	1.00	46.53	A
2081	CZ	ARG	A1276	-37.266	-14.682	10.912	1.00	46.62	A
2082	NH1	ARG	A1276	-36.189	-15.484	10.799	1.00	41.73	A
2083	NH2	ARG	A1276	-37.068	-13.427	10.782	1.00	48.05	A
2084	C	ARG	A1276	-40.697	-19.894	14.480	1.00	60.22	A
2085	O	ARG	A1276	-39.948	-20.831	14.476	1.00	60.07	A
2086	N	GLN	A1277	-42.012	-19.989	14.242	1.00	63.04	A
2087	CA	GLN	A1277	-42.584	-21.287	14.117	1.00	65.55	A
2088	CB	GLN	A1277	-41.896	-22.137	13.025	1.00	64.18	A
2089	CG	GLN	A1277	-42.628	-22.109	11.576	1.00	67.64	A
2090	CD	GLN	A1277	-44.213	-21.898	11.594	1.00	63.83	A
2091	OE1	GLN	A1277	-44.973	-22.754	12.130	1.00	61.97	A
2092	NE2	GLN	A1277	-44.671	-20.752	11.047	1.00	48.65	A
2093	C	GLN	A1277	-42.405	-21.831	15.553	1.00	67.86	A
2094	O	GLN	A1277	-41.829	-22.920	15.749	1.00	68.82	A
2095	N	THR	A1278	-42.976	-21.054	16.489	1.00	69.24	A
2096	CA	THR	A1278	-42.657	-20.977	17.891	1.00	70.98	A
2097	CB	THR	A1278	-43.385	-19.774	18.675	1.00	70.64	A
2098	OG1	THR	A1278	-42.764	-19.547	19.946	1.00	64.44	A
2099	CG2	THR	A1278	-44.835	-20.048	18.836	1.00	67.76	A
2100	C	THR	A1278	-42.880	-22.215	18.701	1.00	74.06	A
2101	O	THR	A1278	-42.569	-23.352	18.262	1.00	76.04	A
2102	N	MET	A1279	-43.345	-22.011	19.939	1.00	74.15	A
2103	CA	MET	A1279	-43.349	-23.158	20.808	1.00	73.96	A
2104	CB	MET	A1279	-43.710	-24.451	19.989	1.00	71.91	A
2105	CG	MET	A1279	-44.639	-25.455	20.658	1.00	70.67	A
2106	SD	MET	A1279	-45.796	-24.779	21.915	1.00	64.86	A
2107	CE	MET	A1279	-46.733	-26.264	22.135	1.00	60.46	A
2108	C	MET	A1279	-41.944	-23.196	21.506	1.00	73.87	A
2109	O	MET	A1279	-41.695	-22.328	22.406	1.00	74.09	A
2110	N	ASP	A1280	-41.081	-24.173	21.127	1.00	71.79	A
2111	CA	ASP	A1280	-39.974	-24.713	21.988	1.00	69.68	A
2112	CB	ASP	A1280	-39.983	-26.287	22.152	1.00	69.86	A
2113	CG	ASP	A1280	-41.448	-26.932	22.461	1.00	72.10	A
2114	OD1	ASP	A1280	-42.394	-26.757	21.632	1.00	75.65	A
2115	OD2	ASP	A1280	-41.693	-27.649	23.513	1.00	70.69	A

2116	C	ASP	A1280	-38.841	-24.225	21.157	1.00	69.93	A
2117	O	ASP	A1280	-38.982	-23.185	20.494	1.00	71.89	A
2118	N	LEU	A1281	-37.732	-24.941	21.038	1.00	69.08	A
2119	CA	LEU	A1281	-36.681	-24.364	20.180	1.00	66.54	A
2120	CB	LEU	A1281	-35.587	-23.647	21.037	1.00	64.84	A
2121	CG	LEU	A1281	-35.981	-22.350	21.746	1.00	65.58	A
2122	CD1	LEU	A1281	-35.232	-21.955	23.025	1.00	68.09	A
2123	CD2	LEU	A1281	-35.863	-21.269	20.846	1.00	65.17	A
2124	C	LEU	A1281	-36.099	-25.301	19.048	1.00	65.78	A
2125	O	LEU	A1281	-35.750	-26.458	19.234	1.00	64.93	A
2126	N	SER	A1282	-35.967	-24.729	17.873	1.00	65.34	A
2127	CA	SER	A1282	-35.545	-25.451	16.684	1.00	64.85	A
2128	CB	SER	A1282	-36.740	-25.945	15.860	1.00	65.16	A
2129	OG	SER	A1282	-37.767	-24.925	15.691	1.00	66.46	A
2130	C	SER	A1282	-34.781	-24.423	15.852	1.00	63.77	A
2131	O	SER	A1282	-35.369	-23.420	15.417	1.00	60.98	A
2132	N	ALA	A1283	-33.466	-24.707	15.724	1.00	61.86	A
2133	CA	ALA	A1283	-32.610	-24.151	14.749	1.00	59.12	A
2134	CB	ALA	A1283	-31.297	-24.642	14.954	1.00	59.47	A
2135	C	ALA	A1283	-33.124	-24.748	13.477	1.00	58.43	A
2136	O	ALA	A1283	-32.447	-25.734	12.965	1.00	56.69	A
2137	N	ASN	A1284	-34.226	-24.113	13.011	1.00	55.91	A
2138	CA	ASN	A1284	-34.880	-24.195	11.681	1.00	57.17	A
2139	CB	ASN	A1284	-36.376	-24.164	11.915	1.00	57.94	A
2140	CG	ASN	A1284	-36.714	-23.124	12.906	1.00	57.22	A
2141	OD1	ASN	A1284	-35.831	-22.426	13.331	1.00	54.31	A
2142	ND2	ASN	A1284	-37.915	-23.092	13.369	1.00	57.18	A
2143	C	ASN	A1284	-34.621	-23.037	10.688	1.00	57.75	A
2144	O	ASN	A1284	-34.134	-23.296	9.579	1.00	60.33	A
2145	N	GLN	A1285	-35.044	-21.802	10.984	1.00	57.48	A
2146	CA	GLN	A1285	-34.458	-20.549	10.261	1.00	56.05	A
2147	CB	GLN	A1285	-34.932	-19.164	10.761	1.00	54.06	A
2148	CG	GLN	A1285	-36.364	-19.127	11.317	1.00	52.12	A
2149	CD	GLN	A1285	-37.331	-19.696	10.379	1.00	45.75	A
2150	OE1	GLN	A1285	-37.161	-19.573	9.167	1.00	56.75	A
2151	NE2	GLN	A1285	-38.416	-20.162	10.880	1.00	44.35	A
2152	C	GLN	A1285	-32.991	-20.456	10.079	1.00	54.52	A
2153	O	GLN	A1285	-32.251	-21.191	10.644	1.00	55.07	A
2154	N	ASP	A1286	-32.617	-19.468	9.278	1.00	55.60	A
2155	CA	ASP	A1286	-31.264	-19.260	8.753	1.00	55.76	A
2156	CB	ASP	A1286	-30.860	-20.208	7.601	1.00	56.69	A
2157	CG	ASP	A1286	-31.524	-19.846	6.292	1.00	57.05	A
2158	OD1	ASP	A1286	-30.762	-19.594	5.332	1.00	51.80	A
2159	OD2	ASP	A1286	-32.801	-19.826	6.207	1.00	62.40	A
2160	C	ASP	A1286	-31.090	-17.895	8.237	1.00	55.77	A
2161	O	ASP	A1286	-30.385	-17.742	7.256	1.00	56.28	A
2162	N	GLU	A1287	-31.708	-16.960	8.937	1.00	55.51	A
2163	CA	GLU	A1287	-31.438	-15.516	9.009	1.00	57.62	A
2164	CB	GLU	A1287	-32.761	-14.753	8.673	1.00	56.24	A
2165	CG	GLU	A1287	-33.027	-14.812	7.237	1.00	63.46	A
2166	CD	GLU	A1287	-34.463	-15.040	6.835	1.00	67.81	A
2167	OE1	GLU	A1287	-34.735	-16.170	6.266	1.00	62.06	A
2168	OE2	GLU	A1287	-35.270	-14.068	7.061	1.00	70.34	A
2169	C	GLU	A1287	-31.027	-15.068	10.490	1.00	57.64	A
2170	O	GLU	A1287	-31.153	-15.878	11.432	1.00	59.88	A
2171	N	GLU	A1288	-30.772	-13.772	10.684	1.00	54.37	A

2172	CA	GLU	A1288	-30.322	-13.205	11.902	1.00	54.07	A
2173	CB	GLU	A1288	-28.928	-12.676	11.656	1.00	56.10	A
2174	CG	GLU	A1288	-27.838	-13.348	12.506	1.00	56.86	A
2175	CD	GLU	A1288	-26.614	-13.537	11.705	1.00	60.27	A
2176	OE1	GLU	A1288	-25.727	-12.640	11.908	1.00	66.32	A
2177	OE2	GLU	A1288	-26.503	-14.556	10.880	1.00	57.45	A
2178	C	GLU	A1288	-31.226	-12.018	12.528	1.00	55.17	A
2179	O	GLU	A1288	-30.758	-10.785	12.648	1.00	53.18	A
2180	N	THR	A1289	-32.490	-12.394	12.909	1.00	53.19	A
2181	CA	THR	A1289	-33.515	-11.409	13.238	1.00	52.05	A
2182	CB	THR	A1289	-34.813	-11.718	12.568	1.00	52.81	A
2183	OG1	THR	A1289	-35.339	-12.935	13.227	1.00	55.08	A
2184	CG2	THR	A1289	-34.572	-11.758	11.078	1.00	44.93	A
2185	C	THR	A1289	-33.958	-11.337	14.701	1.00	50.30	A
2186	O	THR	A1289	-33.628	-12.166	15.517	1.00	49.64	A
2187	N	ASP	A1290	-34.733	-10.331	14.997	1.00	47.83	A
2188	CA	ASP	A1290	-35.131	-10.188	16.266	1.00	49.76	A
2189	CB	ASP	A1290	-36.273	-9.130	16.297	1.00	48.10	A
2190	CG	ASP	A1290	-35.740	-7.711	16.473	1.00	47.30	A
2191	OD1	ASP	A1290	-36.268	-6.895	17.202	1.00	50.24	A
2192	OD2	ASP	A1290	-34.640	-7.385	16.013	1.00	51.86	A
2193	C	ASP	A1290	-35.262	-11.629	16.979	1.00	52.84	A
2194	O	ASP	A1290	-34.654	-11.925	17.998	1.00	55.90	A
2195	N	GLN	A1291	-35.857	-12.617	16.352	1.00	53.55	A
2196	CA	GLN	A1291	-35.950	-13.867	17.016	1.00	50.92	A
2197	CB	GLN	A1291	-37.291	-14.412	16.762	1.00	51.41	A
2198	CG	GLN	A1291	-38.256	-13.339	16.373	1.00	51.45	A
2199	CD	GLN	A1291	-39.439	-13.933	15.680	1.00	61.15	A
2200	OE1	GLN	A1291	-40.576	-13.846	16.148	1.00	63.10	A
2201	NE2	GLN	A1291	-39.166	-14.648	14.584	1.00	65.14	A
2202	C	GLN	A1291	-34.934	-14.912	16.635	1.00	50.34	A
2203	O	GLN	A1291	-35.161	-16.121	16.868	1.00	51.88	A
2204	N	GLU	A1292	-33.775	-14.536	16.189	1.00	47.41	A
2205	CA	GLU	A1292	-32.675	-15.466	16.326	1.00	47.17	A
2206	CB	GLU	A1292	-32.133	-15.935	14.982	1.00	47.90	A
2207	CG	GLU	A1292	-33.083	-16.675	14.013	1.00	52.12	A
2208	CD	GLU	A1292	-34.361	-15.860	13.514	1.00	61.13	A
2209	OE1	GLU	A1292	-35.514	-16.460	13.685	1.00	52.07	A
2210	OE2	GLU	A1292	-34.184	-14.672	12.953	1.00	54.40	A
2211	C	GLU	A1292	-31.646	-14.609	17.112	1.00	46.86	A
2212	O	GLU	A1292	-30.590	-14.318	16.639	1.00	48.49	A
2213	N	THR	A1293	-32.018	-14.029	18.231	1.00	44.59	A
2214	CA	THR	A1293	-31.106	-13.007	18.754	1.00	42.53	A
2215	CB	THR	A1293	-31.301	-11.651	18.074	1.00	42.24	A
2216	OG1	THR	A1293	-30.591	-11.713	16.853	1.00	44.50	A
2217	CG2	THR	A1293	-30.855	-10.499	18.908	1.00	33.85	A
2218	C	THR	A1293	-31.307	-13.000	20.261	1.00	42.79	A
2219	O	THR	A1293	-32.409	-12.769	20.646	1.00	39.63	A
2220	N	PHE	A1294	-30.270	-13.358	21.063	1.00	41.49	A
2221	CA	PHE	A1294	-30.599	-13.917	22.424	1.00	43.96	A
2222	CB	PHE	A1294	-30.448	-15.506	22.575	1.00	43.77	A
2223	CG	PHE	A1294	-31.331	-16.243	21.608	1.00	44.21	A
2224	CD1	PHE	A1294	-30.835	-16.738	20.399	1.00	35.52	A
2225	CD2	PHE	A1294	-32.744	-16.224	21.769	1.00	45.34	A
2226	CE1	PHE	A1294	-31.771	-17.263	19.425	1.00	36.32	A
2227	CE2	PHE	A1294	-33.590	-16.819	20.738	1.00	41.54	A

2228	CZ	PHE	A1294	-33.063	-17.250	19.622	1.00	31.86	A
2229	C	PHE	A1294	-29.643	-13.233	23.318	1.00	43.75	A
2230	O	PHE	A1294	-28.393	-13.211	23.036	1.00	47.31	A
2231	N	GLN	A1295	-30.204	-12.596	24.309	1.00	40.73	A
2232	CA	GLN	A1295	-29.450	-11.802	25.167	1.00	42.12	A
2233	CB	GLN	A1295	-30.276	-10.881	25.976	1.00	41.58	A
2234	CG	GLN	A1295	-29.363	-9.930	26.744	1.00	44.53	A
2235	CD	GLN	A1295	-30.150	-8.759	27.195	1.00	41.71	A
2236	OE1	GLN	A1295	-30.154	-7.720	26.537	1.00	42.91	A
2237	NE2	GLN	A1295	-30.991	-8.986	28.219	1.00	40.72	A
2238	C	GLN	A1295	-28.829	-12.748	26.081	1.00	45.58	A
2239	O	GLN	A1295	-29.510	-13.240	27.104	1.00	45.84	A
2240	N	LEU	A1296	-27.519	-13.001	25.753	1.00	46.03	A
2241	CA	LEU	A1296	-26.681	-13.921	26.570	1.00	46.37	A
2242	CB	LEU	A1296	-25.339	-14.143	25.839	1.00	44.21	A
2243	CG	LEU	A1296	-24.200	-14.913	26.483	1.00	42.90	A
2244	CD1	LEU	A1296	-23.374	-15.649	25.553	1.00	44.17	A
2245	CD2	LEU	A1296	-23.233	-14.144	27.293	1.00	41.35	A
2246	C	LEU	A1296	-26.504	-13.285	28.054	1.00	46.39	A
2247	O	LEU	A1296	-25.514	-12.507	28.331	1.00	43.57	A
2248	N	GLU	A1297	-27.457	-13.581	28.935	1.00	45.35	A
2249	CA	GLU	A1297	-27.269	-13.151	30.367	1.00	52.41	A
2250	CB	GLU	A1297	-28.580	-13.158	31.227	1.00	51.95	A
2251	CG	GLU	A1297	-29.905	-13.086	30.440	1.00	57.22	A
2252	CD	GLU	A1297	-30.944	-12.307	31.147	1.00	57.00	A
2253	OE1	GLU	A1297	-30.474	-11.577	32.054	1.00	53.53	A
2254	OE2	GLU	A1297	-32.163	-12.480	30.820	1.00	53.79	A
2255	C	GLU	A1297	-26.251	-13.959	31.187	1.00	53.02	A
2256	O	GLU	A1297	-26.619	-14.985	31.640	1.00	56.17	A
2257	N	ILE	A1298	-25.037	-13.542	31.397	1.00	53.74	A
2258	CA	ILE	A1298	-24.100	-14.351	32.279	1.00	55.23	A
2259	CB	ILE	A1298	-22.673	-14.519	31.659	1.00	52.61	A
2260	CG2	ILE	A1298	-21.885	-15.349	32.517	1.00	53.99	A
2261	CG1	ILE	A1298	-22.686	-15.486	30.488	1.00	56.27	A
2262	CD1	ILE	A1298	-21.529	-15.375	29.439	1.00	52.33	A
2263	C	ILE	A1298	-23.913	-13.825	33.752	1.00	54.63	A
2264	O	ILE	A1298	-22.770	-13.582	34.149	1.00	55.67	A
2265	N	ASP	A1299	-24.992	-13.540	34.460	1.00	56.07	A
2266	CA	ASP	A1299	-25.043	-13.267	35.969	1.00	60.33	A
2267	CB	ASP	A1299	-26.221	-14.008	36.642	1.00	62.12	A
2268	CG	ASP	A1299	-25.752	-15.365	37.297	1.00	62.62	A
2269	OD1	ASP	A1299	-25.062	-16.194	36.605	1.00	63.43	A
2270	OD2	ASP	A1299	-26.066	-15.571	38.506	1.00	60.45	A
2271	C	ASP	A1299	-23.849	-13.573	36.928	1.00	61.96	A
2272	O	ASP	A1299	-23.051	-14.656	36.907	1.00	61.35	A
2273	N	ARG	A1300	-23.789	-12.645	37.849	1.00	63.14	A
2274	CA	ARG	A1300	-22.528	-12.577	38.575	1.00	63.13	A
2275	CB	ARG	A1300	-22.409	-11.204	39.274	1.00	65.44	A
2276	CG	ARG	A1300	-21.945	-10.025	38.206	1.00	62.76	A
2277	CD	ARG	A1300	-22.535	-8.592	38.351	1.00	54.72	A
2278	NE	ARG	A1300	-23.884	-8.722	38.904	1.00	50.16	A
2279	CZ	ARG	A1300	-24.799	-7.745	39.025	1.00	48.12	A
2280	NH1	ARG	A1300	-24.607	-6.445	38.667	1.00	39.06	A
2281	NH2	ARG	A1300	-25.900	-8.138	39.530	1.00	48.47	A
2282	C	ARG	A1300	-22.237	-13.911	39.372	1.00	63.91	A
2283	O	ARG	A1300	-21.129	-14.508	39.211	1.00	61.70	A

2284	N	ASP	A1301	-23.289	-14.421	40.040	1.00	63.49	A
2285	CA	ASP	A1301	-23.254	-15.663	40.878	1.00	63.08	A
2286	CB	ASP	A1301	-24.625	-16.135	41.531	1.00	62.65	A
2287	CG	ASP	A1301	-25.772	-15.027	41.605	1.00	65.06	A
2288	OD1	ASP	A1301	-26.990	-15.538	41.803	1.00	64.87	A
2289	OD2	ASP	A1301	-25.465	-13.741	41.461	1.00	56.19	A
2290	C	ASP	A1301	-22.812	-16.873	40.088	1.00	62.74	A
2291	O	ASP	A1301	-21.649	-16.905	39.665	1.00	61.99	A
2292	N	THR	A1302	-23.737	-17.891	40.081	1.00	62.04	A
2293	CA	THR	A1302	-23.772	-19.140	39.351	1.00	60.33	A
2294	CB	THR	A1302	-25.244	-19.400	38.572	1.00	62.02	A
2295	OG1	THR	A1302	-25.278	-18.828	37.267	1.00	60.51	A
2296	CG2	THR	A1302	-26.532	-18.938	39.309	1.00	62.03	A
2297	C	THR	A1302	-22.759	-19.119	38.253	1.00	61.08	A
2298	O	THR	A1302	-22.071	-20.214	37.930	1.00	57.20	A
2299	N	LYS	A1303	-22.761	-17.882	37.623	1.00	61.88	A
2300	CA	LYS	A1303	-21.915	-17.489	36.457	1.00	61.60	A
2301	CB	LYS	A1303	-20.461	-17.961	36.748	1.00	61.48	A
2302	CG	LYS	A1303	-19.159	-16.992	36.765	1.00	61.02	A
2303	CD	LYS	A1303	-19.175	-15.873	37.942	1.00	57.72	A
2304	CE	LYS	A1303	-17.802	-15.283	38.045	1.00	57.92	A
2305	NZ	LYS	A1303	-17.776	-13.840	37.844	1.00	61.12	A
2306	C	LYS	A1303	-22.491	-18.368	35.289	1.00	62.85	A
2307	O	LYS	A1303	-21.759	-18.698	34.362	1.00	62.28	A
2308	N	LYS	A1304	-23.788	-18.751	35.351	1.00	62.95	A
2309	CA	LYS	A1304	-24.346	-19.688	34.406	1.00	64.20	A
2310	CB	LYS	A1304	-25.439	-20.581	35.034	1.00	66.25	A
2311	CG	LYS	A1304	-25.023	-22.019	35.625	1.00	64.38	A
2312	CD	LYS	A1304	-26.041	-22.450	36.735	1.00	65.86	A
2313	CE	LYS	A1304	-26.317	-24.030	36.786	1.00	66.63	A
2314	NZ	LYS	A1304	-25.048	-24.859	36.863	1.00	65.05	A
2315	C	LYS	A1304	-24.755	-18.854	33.166	1.00	64.10	A
2316	O	LYS	A1304	-24.168	-17.813	33.016	1.00	66.49	A
2317	N	CYS	A1305	-25.548	-19.322	32.198	1.00	61.89	A
2318	CA	CYS	A1305	-25.883	-18.471	31.092	1.00	59.45	A
2319	CB	CYS	A1305	-25.130	-18.845	29.883	1.00	59.40	A
2320	SG	CYS	A1305	-25.649	-17.757	28.366	1.00	60.99	A
2321	C	CYS	A1305	-27.369	-18.576	30.785	1.00	59.73	A
2322	O	CYS	A1305	-27.884	-19.747	30.599	1.00	60.28	A
2323	N	ALA	A1306	-28.080	-17.428	30.742	1.00	56.64	A
2324	CA	ALA	A1306	-29.483	-17.550	30.632	1.00	55.01	A
2325	CB	ALA	A1306	-30.142	-17.174	31.880	1.00	54.82	A
2326	C	ALA	A1306	-30.199	-16.929	29.464	1.00	54.76	A
2327	O	ALA	A1306	-31.073	-16.138	29.707	1.00	57.78	A
2328	N	PHE	A1307	-29.943	-17.329	28.226	1.00	51.55	A
2329	CA	PHE	A1307	-30.506	-16.597	27.096	1.00	50.57	A
2330	CB	PHE	A1307	-30.454	-17.490	25.859	1.00	48.35	A
2331	CG	PHE	A1307	-29.040	-18.104	25.604	1.00	44.69	A
2332	CD1	PHE	A1307	-28.819	-19.380	25.732	1.00	30.80	A
2333	CD2	PHE	A1307	-27.973	-17.349	25.181	1.00	44.28	A
2334	CE1	PHE	A1307	-27.639	-19.864	25.385	1.00	38.00	A
2335	CE2	PHE	A1307	-26.760	-17.857	24.931	1.00	37.31	A
2336	CZ	PHE	A1307	-26.572	-19.105	25.003	1.00	35.33	A
2337	C	PHE	A1307	-31.919	-15.896	27.272	1.00	49.78	A
2338	O	PHE	A1307	-32.832	-16.606	27.675	1.00	53.55	A
2339	N	ARG	A1308	-32.092	-14.575	27.051	1.00	45.29	A

2340	CA	ARG	A1308	-33.387	-13.972	27.132	1.00	45.96	A
2341	CB	ARG	A1308	-33.272	-12.511	27.487	1.00	46.09	A
2342	CG	ARG	A1308	-34.006	-11.885	28.709	1.00	38.83	A
2343	CD	ARG	A1308	-35.390	-12.015	28.519	1.00	38.95	A
2344	NE	ARG	A1308	-35.947	-10.887	29.264	1.00	45.19	A
2345	CZ	ARG	A1308	-35.449	-9.658	29.230	1.00	48.02	A
2346	NH1	ARG	A1308	-34.530	-9.364	28.360	1.00	48.04	A
2347	NH2	ARG	A1308	-35.990	-8.674	29.943	1.00	53.38	A
2348	C	ARG	A1308	-33.888	-13.926	25.742	1.00	46.75	A
2349	O	ARG	A1308	-33.116	-13.783	24.923	1.00	47.35	A
2350	N	THR	A1309	-35.194	-13.944	25.446	1.00	48.50	A
2351	CA	THR	A1309	-35.782	-13.836	24.023	1.00	47.11	A
2352	CB	THR	A1309	-36.903	-14.811	23.938	1.00	45.73	A
2353	OG1	THR	A1309	-37.894	-14.369	24.912	1.00	48.67	A
2354	CG2	THR	A1309	-36.495	-16.233	24.359	1.00	40.34	A
2355	C	THR	A1309	-36.399	-12.306	23.903	1.00	47.28	A
2356	O	THR	A1309	-36.668	-11.666	24.968	1.00	47.89	A
2357	N	HIS	A1310	-36.606	-11.728	22.701	1.00	45.42	A
2358	CA	HIS	A1310	-37.246	-10.416	22.569	1.00	46.98	A
2359	CB	HIS	A1310	-37.336	-9.953	21.146	1.00	45.07	A
2360	CG	HIS	A1310	-38.080	-10.909	20.289	1.00	46.29	A
2361	CD2	HIS	A1310	-37.719	-12.141	19.840	1.00	47.63	A
2362	ND1	HIS	A1310	-39.409	-10.711	19.893	1.00	49.66	A
2363	CE1	HIS	A1310	-39.835	-11.786	19.224	1.00	46.35	A
2364	NE2	HIS	A1310	-38.845	-12.683	19.229	1.00	54.25	A
2365	C	HIS	A1310	-38.663	-10.431	23.049	1.00	52.14	A
2366	O	HIS	A1310	-39.159	-9.336	23.489	1.00	57.70	A
2367	N	THR	A1311	-39.413	-11.555	22.991	1.00	53.67	A
2368	CA	THR	A1311	-40.762	-11.508	23.610	1.00	52.16	A
2369	CB	THR	A1311	-41.300	-12.936	23.433	1.00	54.44	A
2370	OG1	THR	A1311	-41.387	-13.596	24.751	1.00	54.84	A
2371	CG2	THR	A1311	-40.432	-13.716	22.519	1.00	40.18	A
2372	C	THR	A1311	-40.638	-11.294	25.225	1.00	52.76	A
2373	O	THR	A1311	-41.574	-11.335	25.966	1.00	51.73	A
2374	N	GLY	A1312	-39.430	-11.200	25.767	1.00	53.22	A
2375	CA	GLY	A1312	-39.245	-11.201	27.232	1.00	53.65	A
2376	C	GLY	A1312	-39.285	-12.557	28.000	1.00	55.17	A
2377	O	GLY	A1312	-39.739	-12.545	29.162	1.00	56.16	A
2378	N	LYS	A1313	-38.889	-13.714	27.364	1.00	52.15	A
2379	CA	LYS	A1313	-39.025	-15.073	27.995	1.00	48.68	A
2380	CB	LYS	A1313	-40.026	-15.963	27.399	1.00	44.37	A
2381	CG	LYS	A1313	-41.329	-15.720	28.042	1.00	41.73	A
2382	CD	LYS	A1313	-41.800	-14.245	27.801	1.00	37.92	A
2383	CE	LYS	A1313	-42.938	-13.729	28.699	1.00	36.62	A
2384	NZ	LYS	A1313	-44.013	-14.677	28.388	1.00	36.38	A
2385	C	LYS	A1313	-37.702	-15.624	27.850	1.00	49.51	A
2386	O	LYS	A1313	-36.832	-14.902	27.260	1.00	51.86	A
2387	N	TYR	A1314	-37.482	-16.822	28.416	1.00	47.74	A
2388	CA	TYR	A1314	-36.169	-17.322	28.677	1.00	47.12	A
2389	CB	TYR	A1314	-36.104	-17.397	30.241	1.00	51.07	A
2390	CG	TYR	A1314	-35.644	-16.104	30.800	1.00	54.48	A
2391	CD1	TYR	A1314	-36.579	-15.041	31.039	1.00	56.56	A
2392	CE1	TYR	A1314	-36.102	-13.752	31.537	1.00	54.73	A
2393	CD2	TYR	A1314	-34.211	-15.834	30.937	1.00	54.49	A
2394	CE2	TYR	A1314	-33.743	-14.524	31.385	1.00	49.88	A
2395	CZ	TYR	A1314	-34.679	-13.534	31.727	1.00	50.77	A

2396	OH	TYR	A1314	-34.216	-12.300	32.128	1.00	48.25	A
2397	C	TYR	A1314	-36.050	-18.669	28.113	1.00	46.35	A
2398	O	TYR	A1314	-37.071	-19.396	27.987	1.00	47.04	A
2399	N	TRP	A1315	-34.845	-19.066	27.708	1.00	45.60	A
2400	CA	TRP	A1315	-34.715	-20.496	27.297	1.00	45.58	A
2401	CB	TRP	A1315	-33.423	-20.857	26.670	1.00	40.95	A
2402	CG	TRP	A1315	-33.174	-20.302	25.469	1.00	38.61	A
2403	CD2	TRP	A1315	-32.311	-20.871	24.444	1.00	34.25	A
2404	CE2	TRP	A1315	-32.379	-20.065	23.354	1.00	33.27	A
2405	CE3	TRP	A1315	-31.381	-21.883	24.432	1.00	33.32	A
2406	CD1	TRP	A1315	-33.728	-19.187	24.944	1.00	33.92	A
2407	NE1	TRP	A1315	-33.242	-19.024	23.658	1.00	33.24	A
2408	CZ2	TRP	A1315	-31.430	-20.207	22.250	1.00	37.03	A
2409	CZ3	TRP	A1315	-30.623	-22.144	23.292	1.00	31.61	A
2410	CH2	TRP	A1315	-30.675	-21.271	22.178	1.00	30.47	A
2411	C	TRP	A1315	-34.804	-21.347	28.597	1.00	49.38	A
2412	O	TRP	A1315	-33.948	-21.188	29.539	1.00	47.10	A
2413	N	THR	A1316	-35.862	-22.195	28.586	1.00	52.15	A
2414	CA	THR	A1316	-36.332	-23.035	29.755	1.00	53.79	A
2415	CB	THR	A1316	-37.843	-22.930	30.052	1.00	51.85	A
2416	OG1	THR	A1316	-38.156	-21.581	30.401	1.00	55.16	A
2417	CG2	THR	A1316	-38.103	-23.600	31.269	1.00	54.88	A
2418	C	THR	A1316	-35.973	-24.498	29.491	1.00	53.04	A
2419	O	THR	A1316	-35.158	-24.737	28.580	1.00	52.01	A
2420	N	LEU	A1317	-36.472	-25.425	30.330	1.00	53.12	A
2421	CA	LEU	A1317	-36.255	-26.864	30.080	1.00	55.15	A
2422	CB	LEU	A1317	-34.977	-27.435	30.749	1.00	58.03	A
2423	CG	LEU	A1317	-34.627	-28.898	31.021	1.00	55.21	A
2424	CD1	LEU	A1317	-33.443	-28.802	31.949	1.00	46.05	A
2425	CD2	LEU	A1317	-35.915	-29.571	31.723	1.00	58.28	A
2426	C	LEU	A1317	-37.451	-27.645	30.366	1.00	54.46	A
2427	O	LEU	A1317	-38.180	-27.342	31.227	1.00	54.11	A
2428	N	THR	A1318	-37.687	-28.584	29.489	1.00	57.29	A
2429	CA	THR	A1318	-38.900	-29.373	29.476	1.00	57.17	A
2430	CB	THR	A1318	-39.554	-29.522	28.020	1.00	57.20	A
2431	OG1	THR	A1318	-38.549	-29.503	27.013	1.00	54.08	A
2432	CG2	THR	A1318	-40.539	-28.472	27.704	1.00	53.93	A
2433	C	THR	A1318	-38.391	-30.726	29.938	1.00	57.85	A
2434	O	THR	A1318	-37.243	-31.135	29.692	1.00	58.03	A
2435	N	ALA	A1319	-39.291	-31.417	30.599	1.00	59.71	A
2436	CA	ALA	A1319	-39.134	-32.818	30.956	1.00	59.65	A
2437	CB	ALA	A1319	-40.238	-33.227	31.550	1.00	59.23	A
2438	C	ALA	A1319	-38.827	-33.742	29.862	1.00	60.09	A
2439	O	ALA	A1319	-38.223	-34.684	30.131	1.00	63.86	A
2440	N	THR	A1320	-39.178	-33.526	28.616	1.00	62.14	A
2441	CA	THR	A1320	-38.541	-34.365	27.512	1.00	62.88	A
2442	CB	THR	A1320	-39.282	-34.245	26.122	1.00	62.06	A
2443	OG1	THR	A1320	-40.659	-34.394	26.380	1.00	59.63	A
2444	CG2	THR	A1320	-38.861	-35.273	25.111	1.00	59.74	A
2445	C	THR	A1320	-37.055	-34.122	27.378	1.00	63.36	A
2446	O	THR	A1320	-36.258	-34.992	27.535	1.00	64.27	A
2447	N	GLY	A1321	-36.726	-32.882	27.184	1.00	66.19	A
2448	CA	GLY	A1321	-35.375	-32.371	27.159	1.00	67.99	A
2449	C	GLY	A1321	-35.571	-31.355	26.068	1.00	69.77	A
2450	O	GLY	A1321	-34.750	-31.246	25.150	1.00	71.91	A
2451	N	GLY	A1322	-36.698	-30.629	26.139	1.00	70.04	A

2452	CA	GLY	A1322	-36.988	-29.637	25.168	1.00	68.10	A
2453	C	GLY	A1322	-36.614	-28.299	25.767	1.00	68.18	A
2454	O	GLY	A1322	-37.044	-27.918	26.860	1.00	68.03	A
2455	N	VAL	A1323	-35.804	-27.587	24.995	1.00	67.70	A
2456	CA	VAL	A1323	-35.547	-26.221	25.211	1.00	65.63	A
2457	CB	VAL	A1323	-34.137	-25.834	24.749	1.00	65.17	A
2458	CG1	VAL	A1323	-33.788	-24.449	25.342	1.00	69.02	A
2459	CG2	VAL	A1323	-33.170	-26.727	25.300	1.00	57.55	A
2460	C	VAL	A1323	-36.688	-25.516	24.550	1.00	65.49	A
2461	O	VAL	A1323	-36.991	-25.657	23.361	1.00	62.76	A
2462	N	GLN	A1324	-37.427	-24.879	25.418	1.00	66.89	A
2463	CA	GLN	A1324	-38.676	-24.224	24.967	1.00	68.49	A
2464	CB	GLN	A1324	-39.954	-24.887	25.557	1.00	68.64	A
2465	CG	GLN	A1324	-40.316	-24.496	27.109	1.00	73.20	A
2466	CD	GLN	A1324	-41.673	-25.137	27.589	1.00	71.90	A
2467	OE1	GLN	A1324	-42.144	-24.892	28.747	1.00	75.14	A
2468	NE2	GLN	A1324	-42.273	-25.984	26.705	1.00	67.97	A
2469	C	GLN	A1324	-38.586	-22.782	25.325	1.00	66.93	A
2470	O	GLN	A1324	-37.755	-22.370	26.146	1.00	69.80	A
2471	N	SER	A1325	-39.354	-21.950	24.692	1.00	66.19	A
2472	CA	SER	A1325	-38.936	-20.566	24.868	1.00	66.25	A
2473	CB	SER	A1325	-38.517	-19.986	23.514	1.00	65.18	A
2474	OG	SER	A1325	-39.679	-19.461	22.827	1.00	67.74	A
2475	C	SER	A1325	-39.968	-19.748	25.699	1.00	64.07	A
2476	O	SER	A1325	-40.500	-18.778	25.201	1.00	64.07	A
2477	N	THR	A1326	-40.144	-20.141	26.967	1.00	61.78	A
2478	CA	THR	A1326	-41.276	-19.846	27.743	1.00	61.85	A
2479	CB	THR	A1326	-41.892	-21.151	28.001	1.00	63.57	A
2480	OG1	THR	A1326	-43.260	-20.971	28.500	1.00	63.52	A
2481	CG2	THR	A1326	-40.955	-21.938	28.976	1.00	64.05	A
2482	C	THR	A1326	-41.272	-19.034	29.124	1.00	62.45	A
2483	O	THR	A1326	-42.059	-18.148	29.246	1.00	61.71	A
2484	N	ALA	A1327	-40.492	-19.383	30.153	1.00	62.02	A
2485	CA	ALA	A1327	-40.503	-18.749	31.512	1.00	60.65	A
2486	CB	ALA	A1327	-39.168	-19.217	32.321	1.00	59.87	A
2487	C	ALA	A1327	-40.554	-17.248	31.596	1.00	60.60	A
2488	O	ALA	A1327	-39.537	-16.580	31.826	1.00	60.44	A
2489	N	SER	A1328	-41.712	-16.654	31.512	1.00	61.78	A
2490	CA	SER	A1328	-41.687	-15.209	31.745	1.00	62.33	A
2491	CB	SER	A1328	-43.013	-14.619	32.084	1.00	61.54	A
2492	OG	SER	A1328	-43.915	-14.902	31.091	1.00	60.82	A
2493	C	SER	A1328	-40.813	-14.936	32.925	1.00	63.76	A
2494	O	SER	A1328	-39.820	-14.263	32.767	1.00	65.62	A
2495	N	SER	A1329	-41.216	-15.380	34.116	1.00	64.82	A
2496	CA	SER	A1329	-40.383	-15.124	35.281	1.00	64.99	A
2497	CB	SER	A1329	-41.109	-15.198	36.648	1.00	65.44	A
2498	OG	SER	A1329	-42.504	-15.192	36.583	1.00	58.86	A
2499	C	SER	A1329	-39.453	-16.253	35.221	1.00	64.80	A
2500	O	SER	A1329	-40.007	-17.379	35.073	1.00	65.86	A
2501	N	LYS	A1330	-38.131	-15.959	35.434	1.00	63.54	A
2502	CA	LYS	A1330	-36.974	-16.882	35.418	1.00	61.70	A
2503	CB	LYS	A1330	-35.724	-16.119	35.845	1.00	62.33	A
2504	CG	LYS	A1330	-34.997	-15.324	34.659	1.00	62.11	A
2505	CD	LYS	A1330	-33.524	-15.324	34.795	1.00	56.81	A
2506	CE	LYS	A1330	-32.842	-14.044	34.333	1.00	61.29	A
2507	NZ	LYS	A1330	-33.516	-12.612	34.511	1.00	60.55	A

2508	C	LYS	A1330	-37.107	-18.188	36.232	1.00	63.44	A
2509	O	LYS	A1330	-38.236	-18.646	36.542	1.00	63.66	A
2510	N	ASN	A1331	-35.981	-18.870	36.530	1.00	65.06	A
2511	CA	ASN	A1331	-35.995	-20.238	37.095	1.00	64.42	A
2512	CB	ASN	A1331	-37.112	-21.093	36.514	1.00	62.48	A
2513	CG	ASN	A1331	-36.900	-22.629	36.810	1.00	67.38	A
2514	OD1	ASN	A1331	-36.078	-23.312	36.125	1.00	69.59	A
2515	ND2	ASN	A1331	-37.634	-23.191	37.840	1.00	61.93	A
2516	C	ASN	A1331	-34.679	-20.964	36.834	1.00	66.70	A
2517	O	ASN	A1331	-33.678	-20.409	36.251	1.00	68.54	A
2518	N	ALA	A1332	-34.674	-22.230	37.276	1.00	65.78	A
2519	CA	ALA	A1332	-33.560	-23.109	37.111	1.00	63.19	A
2520	CB	ALA	A1332	-33.564	-24.102	38.206	1.00	64.04	A
2521	C	ALA	A1332	-33.596	-23.845	35.807	1.00	62.23	A
2522	O	ALA	A1332	-32.497	-24.196	35.242	1.00	64.30	A
2523	N	SER	A1333	-34.782	-24.222	35.340	1.00	58.06	A
2524	CA	SER	A1333	-34.744	-24.974	34.121	1.00	55.86	A
2525	CB	SER	A1333	-36.068	-25.504	33.621	1.00	53.81	A
2526	OG	SER	A1333	-37.040	-24.543	33.616	1.00	49.75	A
2527	C	SER	A1333	-34.068	-24.192	33.019	1.00	57.62	A
2528	O	SER	A1333	-34.127	-24.696	31.931	1.00	58.13	A
2529	N	CYS	A1334	-33.364	-23.069	33.339	1.00	57.87	A
2530	CA	CYS	A1334	-32.853	-21.993	32.449	1.00	58.83	A
2531	CB	CYS	A1334	-33.441	-20.670	32.890	1.00	58.51	A
2532	SG	CYS	A1334	-35.339	-20.845	32.764	1.00	69.57	A
2533	C	CYS	A1334	-31.359	-21.869	32.291	1.00	57.97	A
2534	O	CYS	A1334	-30.818	-22.054	31.303	1.00	57.85	A
2535	N	TYR	A1335	-30.654	-21.611	33.335	1.00	60.30	A
2536	CA	TYR	A1335	-29.215	-21.777	33.329	1.00	58.08	A
2537	CB	TYR	A1335	-28.795	-21.870	34.760	1.00	59.91	A
2538	CG	TYR	A1335	-29.333	-20.747	35.538	1.00	60.55	A
2539	CD1	TYR	A1335	-30.003	-20.964	36.679	1.00	64.79	A
2540	CE1	TYR	A1335	-30.500	-19.910	37.399	1.00	66.96	A
2541	CD2	TYR	A1335	-29.217	-19.442	35.086	1.00	63.66	A
2542	CE2	TYR	A1335	-29.675	-18.345	35.821	1.00	64.41	A
2543	CZ	TYR	A1335	-30.312	-18.578	36.991	1.00	66.87	A
2544	OH	TYR	A1335	-30.840	-17.474	37.730	1.00	70.42	A
2545	C	TYR	A1335	-28.611	-22.900	32.491	1.00	58.29	A
2546	O	TYR	A1335	-29.307	-23.794	32.067	1.00	60.26	A
2547	N	PHE	A1336	-27.301	-22.781	32.177	1.00	56.15	A
2548	CA	PHE	A1336	-26.532	-23.643	31.179	1.00	50.42	A
2549	CB	PHE	A1336	-26.869	-23.331	29.720	1.00	45.55	A
2550	CG	PHE	A1336	-28.232	-23.509	29.380	1.00	40.17	A
2551	CD1	PHE	A1336	-28.654	-24.634	28.881	1.00	40.89	A
2552	CD2	PHE	A1336	-29.136	-22.492	29.428	1.00	41.13	A
2553	CE1	PHE	A1336	-29.996	-24.783	28.483	1.00	33.95	A
2554	CE2	PHE	A1336	-30.492	-22.708	29.021	1.00	26.67	A
2555	CZ	PHE	A1336	-30.874	-23.877	28.693	1.00	31.66	A
2556	C	PHE	A1336	-25.146	-23.156	31.385	1.00	47.56	A
2557	O	PHE	A1336	-24.989	-21.985	31.748	1.00	47.15	A
2558	N	ASP	A1337	-24.214	-24.054	31.173	1.00	45.85	A
2559	CA	ASP	A1337	-22.814	-23.845	31.240	1.00	46.34	A
2560	CB	ASP	A1337	-22.139	-24.819	32.169	1.00	45.98	A
2561	CG	ASP	A1337	-23.013	-25.026	33.535	1.00	51.61	A
2562	OD1	ASP	A1337	-23.100	-26.211	34.055	1.00	44.12	A
2563	OD2	ASP	A1337	-23.629	-23.982	33.998	1.00	45.14	A

2564	C	ASP	A1337	-22.427	-24.163	29.901	1.00	48.11	A
2565	O	ASP	A1337	-22.780	-25.186	29.282	1.00	49.94	A
2566	N	ILE	A1338	-21.631	-23.243	29.470	1.00	48.80	A
2567	CA	ILE	A1338	-21.127	-23.197	28.261	1.00	48.93	A
2568	CB	ILE	A1338	-20.900	-21.719	27.990	1.00	49.42	A
2569	CG2	ILE	A1338	-19.987	-21.441	26.783	1.00	54.39	A
2570	CG1	ILE	A1338	-22.158	-21.024	27.591	1.00	48.37	A
2571	CD1	ILE	A1338	-22.938	-20.618	28.704	1.00	44.23	A
2572	C	ILE	A1338	-19.835	-23.761	28.604	1.00	50.17	A
2573	O	ILE	A1338	-19.231	-23.351	29.561	1.00	51.43	A
2574	N	GLU	A1339	-19.378	-24.635	27.727	1.00	53.83	A
2575	CA	GLU	A1339	-17.959	-25.079	27.469	1.00	54.30	A
2576	CB	GLU	A1339	-18.127	-26.628	27.264	1.00	54.36	A
2577	CG	GLU	A1339	-16.893	-27.495	26.975	1.00	54.17	A
2578	CD	GLU	A1339	-17.355	-28.858	26.803	1.00	56.08	A
2579	OE1	GLU	A1339	-18.611	-28.926	26.908	1.00	58.76	A
2580	OE2	GLU	A1339	-16.524	-29.817	26.655	1.00	54.05	A
2581	C	GLU	A1339	-17.254	-24.398	26.213	1.00	54.49	A
2582	O	GLU	A1339	-17.472	-24.759	25.042	1.00	56.52	A
2583	N	TRP	A1340	-16.405	-23.412	26.440	1.00	55.66	A
2584	CA	TRP	A1340	-15.752	-22.490	25.417	1.00	53.15	A
2585	CB	TRP	A1340	-15.096	-21.167	26.093	1.00	51.55	A
2586	CG	TRP	A1340	-16.134	-20.350	26.970	1.00	51.60	A
2587	CD2	TRP	A1340	-17.123	-19.321	26.468	1.00	47.83	A
2588	CE2	TRP	A1340	-17.903	-18.905	27.590	1.00	49.29	A
2589	CE3	TRP	A1340	-17.397	-18.778	25.209	1.00	37.38	A
2590	CD1	TRP	A1340	-16.326	-20.457	28.285	1.00	44.12	A
2591	NE1	TRP	A1340	-17.403	-19.575	28.680	1.00	44.14	A
2592	CZ2	TRP	A1340	-19.009	-17.958	27.463	1.00	55.28	A
2593	CZ3	TRP	A1340	-18.569	-17.936	25.010	1.00	42.69	A
2594	CH2	TRP	A1340	-19.309	-17.470	26.124	1.00	51.78	A
2595	C	TRP	A1340	-14.743	-23.214	24.612	1.00	52.81	A
2596	O	TRP	A1340	-13.522	-22.963	24.635	1.00	54.03	A
2597	N	ARG	A1341	-15.193	-24.092	23.775	1.00	55.65	A
2598	CA	ARG	A1341	-14.187	-24.763	22.893	1.00	55.98	A
2599	CB	ARG	A1341	-14.724	-26.039	22.335	1.00	57.64	A
2600	CG	ARG	A1341	-15.034	-27.122	23.335	1.00	59.51	A
2601	CD	ARG	A1341	-15.800	-28.121	22.452	1.00	64.66	A
2602	NE	ARG	A1341	-15.124	-29.321	21.929	1.00	68.75	A
2603	CZ	ARG	A1341	-14.712	-29.511	20.656	1.00	74.56	A
2604	NH1	ARG	A1341	-14.793	-28.485	19.770	1.00	68.76	A
2605	NH2	ARG	A1341	-14.245	-30.759	20.237	1.00	70.14	A
2606	C	ARG	A1341	-13.690	-23.910	21.775	1.00	54.75	A
2607	O	ARG	A1341	-13.320	-24.386	20.680	1.00	57.08	A
2608	N	ASP	A1342	-13.612	-22.646	22.134	1.00	51.90	A
2609	CA	ASP	A1342	-13.345	-21.443	21.273	1.00	50.64	A
2610	CB	ASP	A1342	-12.028	-20.699	21.773	1.00	49.44	A
2611	CG	ASP	A1342	-10.859	-21.681	21.825	1.00	53.74	A
2612	OD1	ASP	A1342	-11.088	-22.692	22.478	1.00	63.21	A
2613	OD2	ASP	A1342	-9.787	-21.552	21.194	1.00	56.52	A
2614	C	ASP	A1342	-13.382	-21.621	19.702	1.00	48.40	A
2615	O	ASP	A1342	-12.377	-21.924	19.132	1.00	44.85	A
2616	N	ARG	A1343	-14.538	-21.343	19.076	1.00	46.46	A
2617	CA	ARG	A1343	-14.865	-21.449	17.565	1.00	45.77	A
2618	CB	ARG	A1343	-13.922	-22.329	16.781	1.00	43.51	A
2619	CG	ARG	A1343	-12.804	-21.516	16.185	1.00	44.37	A

2620	CD	ARG	A1343	-12.888	-21.327	14.557	1.00	45.61	A
2621	NE	ARG	A1343	-12.121	-20.221	14.054	1.00	34.77	A
2622	CZ	ARG	A1343	-10.765	-20.171	14.030	1.00	40.11	A
2623	NH1	ARG	A1343	-9.982	-21.188	14.509	1.00	32.49	A
2624	NH2	ARG	A1343	-10.137	-19.091	13.453	1.00	35.12	A
2625	C	ARG	A1343	-16.301	-21.943	17.478	1.00	46.67	A
2626	O	ARG	A1343	-17.148	-21.322	16.880	1.00	47.71	A
2627	N	ARG	A1344	-16.599	-22.994	18.243	1.00	46.99	A
2628	CA	ARG	A1344	-17.942	-23.430	18.509	1.00	46.73	A
2629	CB	ARG	A1344	-18.097	-24.803	18.005	1.00	47.01	A
2630	CG	ARG	A1344	-18.240	-24.689	16.531	1.00	53.81	A
2631	CD	ARG	A1344	-16.895	-24.852	15.739	1.00	64.20	A
2632	NE	ARG	A1344	-17.326	-24.580	14.405	1.00	69.32	A
2633	CZ	ARG	A1344	-17.558	-23.375	13.896	1.00	69.64	A
2634	NH1	ARG	A1344	-18.040	-23.373	12.639	1.00	66.38	A
2635	NH2	ARG	A1344	-17.277	-22.244	14.579	1.00	57.92	A
2636	C	ARG	A1344	-18.007	-23.517	19.983	1.00	46.09	A
2637	O	ARG	A1344	-17.009	-23.392	20.589	1.00	43.47	A
2638	N	ILE	A1345	-19.191	-23.863	20.525	1.00	49.79	A
2639	CA	ILE	A1345	-19.618	-23.983	21.986	1.00	47.28	A
2640	CB	ILE	A1345	-20.314	-22.621	22.275	1.00	48.22	A
2641	CG2	ILE	A1345	-21.983	-22.556	22.481	1.00	43.66	A
2642	CG1	ILE	A1345	-19.444	-21.836	23.228	1.00	44.60	A
2643	CD1	ILE	A1345	-20.345	-21.238	24.256	1.00	52.66	A
2644	C	ILE	A1345	-20.500	-25.240	22.353	1.00	47.76	A
2645	O	ILE	A1345	-20.717	-26.108	21.542	1.00	47.71	A
2646	N	THR	A1346	-20.879	-25.381	23.628	1.00	48.55	A
2647	CA	THR	A1346	-21.665	-26.478	24.142	1.00	47.58	A
2648	CB	THR	A1346	-20.809	-27.524	24.963	1.00	47.95	A
2649	OG1	THR	A1346	-19.575	-27.745	24.323	1.00	47.03	A
2650	CG2	THR	A1346	-21.473	-28.992	24.974	1.00	50.44	A
2651	C	THR	A1346	-22.572	-25.742	25.075	1.00	48.87	A
2652	O	THR	A1346	-22.435	-24.540	25.216	1.00	50.92	A
2653	N	LEU	A1347	-23.495	-26.422	25.735	1.00	48.96	A
2654	CA	LEU	A1347	-24.449	-25.756	26.508	1.00	49.28	A
2655	CB	LEU	A1347	-25.624	-25.274	25.608	1.00	49.21	A
2656	CG	LEU	A1347	-26.126	-23.883	26.132	1.00	47.79	A
2657	CD1	LEU	A1347	-25.091	-23.051	25.671	1.00	45.88	A
2658	CD2	LEU	A1347	-27.407	-23.327	25.601	1.00	47.09	A
2659	C	LEU	A1347	-24.797	-26.903	27.415	1.00	51.68	A
2660	O	LEU	A1347	-25.294	-27.936	26.920	1.00	50.08	A
2661	N	ARG	A1348	-24.436	-26.832	28.738	1.00	53.43	A
2662	CA	ARG	A1348	-24.661	-28.088	29.563	1.00	54.18	A
2663	CB	ARG	A1348	-23.611	-28.409	30.622	1.00	53.34	A
2664	CG	ARG	A1348	-23.596	-29.868	31.201	1.00	51.22	A
2665	CD	ARG	A1348	-23.016	-29.879	32.651	1.00	52.22	A
2666	NE	ARG	A1348	-21.554	-29.717	32.635	1.00	52.76	A
2667	CZ	ARG	A1348	-20.549	-30.512	33.023	1.00	50.60	A
2668	NH1	ARG	A1348	-20.782	-31.682	33.589	1.00	56.73	A
2669	NH2	ARG	A1348	-19.246	-30.117	32.779	1.00	45.15	A
2670	C	ARG	A1348	-25.865	-27.631	30.182	1.00	55.44	A
2671	O	ARG	A1348	-25.821	-26.545	30.727	1.00	57.37	A
2672	N	ALA	A1349	-26.920	-28.422	30.095	1.00	55.73	A
2673	CA	ALA	A1349	-28.238	-28.058	30.614	1.00	56.45	A
2674	CB	ALA	A1349	-29.360	-28.936	29.942	1.00	56.37	A
2675	C	ALA	A1349	-28.379	-28.257	32.062	1.00	57.22	A

2676	O	ALA	A1349	-27.420	-28.465	32.802	1.00	54.98	A
2677	N	SER	A1350	-29.640	-28.268	32.456	1.00	59.48	A
2678	CA	SER	A1350	-29.981	-28.572	33.796	1.00	61.95	A
2679	CB	SER	A1350	-31.211	-27.717	34.099	1.00	62.70	A
2680	OG	SER	A1350	-31.362	-27.532	35.475	1.00	68.52	A
2681	C	SER	A1350	-30.170	-30.156	33.950	1.00	62.81	A
2682	O	SER	A1350	-29.759	-30.750	34.975	1.00	66.06	A
2683	N	ASN	A1351	-30.724	-30.896	32.999	1.00	59.48	A
2684	CA	ASN	A1351	-30.531	-32.280	33.236	1.00	56.89	A
2685	CB	ASN	A1351	-31.495	-33.109	32.416	1.00	57.32	A
2686	CG	ASN	A1351	-31.450	-32.820	30.910	1.00	52.77	A
2687	OD1	ASN	A1351	-30.675	-32.079	30.390	1.00	51.55	A
2688	ND2	ASN	A1351	-32.332	-33.475	30.228	1.00	51.95	A
2689	C	ASN	A1351	-29.050	-32.728	33.099	1.00	58.49	A
2690	O	ASN	A1351	-28.738	-33.903	32.832	1.00	56.41	A
2691	N	GLY	A1352	-28.107	-31.798	33.318	1.00	59.63	A
2692	CA	GLY	A1352	-26.665	-32.067	33.111	1.00	59.95	A
2693	C	GLY	A1352	-26.323	-32.681	31.751	1.00	60.84	A
2694	O	GLY	A1352	-25.125	-32.865	31.414	1.00	60.45	A
2695	N	LYS	A1353	-27.356	-33.061	31.005	1.00	62.37	A
2696	CA	LYS	A1353	-27.251	-33.698	29.628	1.00	64.40	A
2697	CB	LYS	A1353	-28.646	-34.129	29.158	1.00	63.45	A
2698	CG	LYS	A1353	-29.334	-35.076	30.128	1.00	60.26	A
2699	CD	LYS	A1353	-29.141	-36.571	29.794	1.00	51.21	A
2700	CE	LYS	A1353	-29.266	-37.463	30.963	1.00	39.98	A
2701	NZ	LYS	A1353	-30.496	-37.017	31.969	1.00	39.61	A
2702	C	LYS	A1353	-26.747	-32.697	28.585	1.00	65.41	A
2703	O	LYS	A1353	-26.696	-31.492	28.937	1.00	68.97	A
2704	N	PHE	A1354	-26.452	-33.124	27.327	1.00	64.50	A
2705	CA	PHE	A1354	-26.225	-32.125	26.192	1.00	63.23	A
2706	CB	PHE	A1354	-24.838	-32.279	25.546	1.00	63.91	A
2707	CG	PHE	A1354	-23.716	-32.048	26.566	1.00	70.21	A
2708	CD1	PHE	A1354	-23.673	-30.864	27.322	1.00	73.78	A
2709	CD2	PHE	A1354	-22.748	-33.043	26.846	1.00	72.11	A
2710	CE1	PHE	A1354	-22.647	-30.705	28.261	1.00	77.23	A
2711	CE2	PHE	A1354	-21.732	-32.886	27.788	1.00	66.14	A
2712	CZ	PHE	A1354	-21.686	-31.767	28.492	1.00	71.64	A
2713	C	PHE	A1354	-27.340	-31.367	25.325	1.00	60.44	A
2714	O	PHE	A1354	-28.352	-31.891	24.976	1.00	59.27	A
2715	N	VAL	A1355	-27.208	-30.095	25.036	1.00	58.88	A
2716	CA	VAL	A1355	-28.205	-29.609	24.144	1.00	58.29	A
2717	CB	VAL	A1355	-28.497	-28.172	24.305	1.00	60.19	A
2718	CG1	VAL	A1355	-29.412	-27.757	23.171	1.00	57.84	A
2719	CG2	VAL	A1355	-29.090	-27.881	25.788	1.00	56.65	A
2720	C	VAL	A1355	-27.905	-30.015	22.699	1.00	58.93	A
2721	O	VAL	A1355	-26.790	-29.787	22.170	1.00	58.73	A
2722	N	THR	A1356	-28.844	-30.817	22.147	1.00	59.71	A
2723	CA	THR	A1356	-28.761	-31.250	20.716	1.00	58.29	A
2724	CB	THR	A1356	-28.459	-32.836	20.459	1.00	56.92	A
2725	OG1	THR	A1356	-27.265	-32.934	19.586	1.00	54.96	A
2726	CG2	THR	A1356	-29.573	-33.473	19.701	1.00	54.19	A
2727	C	THR	A1356	-29.841	-30.581	19.778	1.00	56.27	A
2728	O	THR	A1356	-30.865	-30.172	20.272	1.00	52.39	A
2729	N	SER	A1357	-29.546	-30.550	18.472	1.00	56.37	A
2730	CA	SER	A1357	-30.489	-30.393	17.329	1.00	59.51	A
2731	CB	SER	A1357	-29.626	-29.735	16.188	1.00	59.21	A

2732	OG	SER	A1357	-28.722	-30.763	15.671	1.00	57.32	A
2733	C	SER	A1357	-31.255	-31.705	16.714	1.00	59.54	A
2734	O	SER	A1357	-30.875	-32.247	15.669	1.00	59.56	A
2735	N	LYS	A1358	-32.310	-32.217	17.301	1.00	59.83	A
2736	CA	LYS	A1358	-33.005	-33.400	16.684	1.00	62.57	A
2737	CB	LYS	A1358	-34.149	-33.964	17.596	1.00	62.50	A
2738	CG	LYS	A1358	-33.810	-34.409	19.102	1.00	63.70	A
2739	CD	LYS	A1358	-34.898	-35.317	19.945	1.00	63.05	A
2740	CE	LYS	A1358	-36.414	-34.984	19.741	1.00	58.01	A
2741	NZ	LYS	A1358	-37.309	-36.176	20.144	1.00	55.33	A
2742	C	LYS	A1358	-33.590	-33.221	15.206	1.00	63.76	A
2743	O	LYS	A1358	-33.949	-32.133	14.716	1.00	61.20	A
2744	N	LYS	A1359	-33.650	-34.343	14.466	1.00	67.46	A
2745	CA	LYS	A1359	-34.259	-34.308	13.103	1.00	67.31	A
2746	CB	LYS	A1359	-34.564	-35.769	12.622	1.00	68.61	A
2747	CG	LYS	A1359	-33.233	-36.733	12.440	1.00	69.22	A
2748	CD	LYS	A1359	-33.375	-38.247	12.876	1.00	66.64	A
2749	CE	LYS	A1359	-34.821	-38.894	12.782	1.00	66.66	A
2750	NZ	LYS	A1359	-35.863	-38.766	13.976	1.00	56.99	A
2751	C	LYS	A1359	-35.501	-33.267	13.134	1.00	68.64	A
2752	O	LYS	A1359	-35.708	-32.435	12.233	1.00	67.27	A
2753	N	ASN	A1360	-36.259	-33.230	14.232	1.00	68.84	A
2754	CA	ASN	A1360	-37.390	-32.281	14.236	1.00	69.53	A
2755	CB	ASN	A1360	-38.417	-32.484	15.392	1.00	69.24	A
2756	CG	ASN	A1360	-37.807	-32.919	16.715	1.00	67.27	A
2757	OD1	ASN	A1360	-37.317	-32.125	17.443	1.00	69.33	A
2758	ND2	ASN	A1360	-37.971	-34.187	17.075	1.00	74.51	A
2759	C	ASN	A1360	-37.002	-30.782	14.131	1.00	68.76	A
2760	O	ASN	A1360	-37.862	-29.904	14.225	1.00	68.66	A
2761	N	GLY	A1361	-35.707	-30.509	14.017	1.00	67.01	A
2762	CA	GLY	A1361	-35.250	-29.172	14.277	1.00	63.70	A
2763	C	GLY	A1361	-34.876	-28.919	15.722	1.00	61.67	A
2764	O	GLY	A1361	-34.062	-28.074	15.963	1.00	61.39	A
2765	N	GLN	A1362	-35.451	-29.619	16.703	1.00	60.09	A
2766	CA	GLN	A1362	-35.673	-28.934	18.028	1.00	60.12	A
2767	CB	GLN	A1362	-37.060	-29.313	18.746	1.00	59.64	A
2768	CG	GLN	A1362	-36.754	-30.424	19.995	1.00	60.06	A
2769	CD	GLN	A1362	-37.686	-30.419	21.160	1.00	56.60	A
2770	OE1	GLN	A1362	-37.811	-29.426	21.896	1.00	60.76	A
2771	NE2	GLN	A1362	-38.385	-31.525	21.336	1.00	53.51	A
2772	C	GLN	A1362	-34.459	-29.086	18.965	1.00	59.18	A
2773	O	GLN	A1362	-33.622	-29.857	18.631	1.00	58.74	A
2774	N	LEU	A1363	-34.449	-28.441	20.138	1.00	59.07	A
2775	CA	LEU	A1363	-33.349	-28.515	21.042	1.00	60.64	A
2776	CB	LEU	A1363	-32.976	-27.160	21.652	1.00	60.07	A
2777	CG	LEU	A1363	-32.746	-25.861	20.821	1.00	58.30	A
2778	CD1	LEU	A1363	-33.011	-24.635	21.760	1.00	52.04	A
2779	CD2	LEU	A1363	-31.469	-25.732	19.939	1.00	45.48	A
2780	C	LEU	A1363	-33.571	-29.488	22.180	1.00	63.17	A
2781	O	LEU	A1363	-34.393	-29.304	23.087	1.00	64.95	A
2782	N	ALA	A1364	-32.739	-30.522	22.148	1.00	64.37	A
2783	CA	ALA	A1364	-32.851	-31.689	22.968	1.00	61.98	A
2784	CB	ALA	A1364	-33.086	-32.814	22.071	1.00	62.73	A
2785	C	ALA	A1364	-31.577	-31.812	23.782	1.00	61.15	A
2786	O	ALA	A1364	-30.441	-32.054	23.313	1.00	57.82	A
2787	N	ALA	A1365	-31.810	-31.390	25.006	1.00	62.12	A

2788	CA	ALA	A1365	-30.918	-31.595	26.183	1.00	61.05	A
2789	CB	ALA	A1365	-31.395	-30.716	27.258	1.00	59.93	A
2790	C	ALA	A1365	-30.908	-33.084	26.665	1.00	59.92	A
2791	O	ALA	A1365	-31.401	-33.449	27.744	1.00	59.86	A
2792	N	SER	A1366	-30.359	-33.946	25.827	1.00	59.25	A
2793	CA	SER	A1366	-30.474	-35.407	25.970	1.00	57.85	A
2794	CB	SER	A1366	-31.135	-35.963	24.744	1.00	57.21	A
2795	OG	SER	A1366	-32.436	-35.427	24.683	1.00	60.14	A
2796	C	SER	A1366	-29.120	-35.966	26.052	1.00	56.90	A
2797	O	SER	A1366	-28.773	-36.563	27.082	1.00	52.77	A
2798	N	VAL	A1367	-28.327	-35.706	25.001	1.00	57.02	A
2799	CA	VAL	A1367	-26.893	-36.151	25.015	1.00	59.38	A
2800	CB	VAL	A1367	-25.997	-35.435	23.978	1.00	59.06	A
2801	CG1	VAL	A1367	-24.973	-36.466	23.402	1.00	58.89	A
2802	CG2	VAL	A1367	-26.805	-34.879	22.804	1.00	58.45	A
2803	C	VAL	A1367	-26.248	-36.203	26.402	1.00	61.66	A
2804	O	VAL	A1367	-26.726	-35.519	27.350	1.00	64.82	A
2805	N	GLU	A1368	-25.229	-37.036	26.618	1.00	62.30	A
2806	CA	GLU	A1368	-24.514	-36.881	27.951	1.00	62.88	A
2807	CB	GLU	A1368	-24.635	-38.090	29.023	1.00	60.14	A
2808	CG	GLU	A1368	-26.064	-38.506	29.278	1.00	59.78	A
2809	CD	GLU	A1368	-26.312	-39.549	30.359	1.00	62.94	A
2810	OE1	GLU	A1368	-27.386	-40.218	30.341	1.00	55.63	A
2811	OE2	GLU	A1368	-25.457	-39.668	31.268	1.00	70.93	A
2812	C	GLU	A1368	-23.066	-36.543	27.637	1.00	63.23	A
2813	O	GLU	A1368	-22.360	-36.257	28.605	1.00	62.99	A
2814	N	THR	A1369	-22.624	-36.662	26.346	1.00	62.54	A
2815	CA	THR	A1369	-21.233	-36.335	25.969	1.00	62.23	A
2816	CB	THR	A1369	-20.442	-37.490	25.497	1.00	63.31	A
2817	OG1	THR	A1369	-21.012	-38.708	26.030	1.00	68.84	A
2818	CG2	THR	A1369	-18.967	-37.302	25.912	1.00	56.11	A
2819	C	THR	A1369	-21.217	-35.363	24.870	1.00	63.01	A
2820	O	THR	A1369	-22.183	-35.321	24.068	1.00	64.84	A
2821	N	ALA	A1370	-20.164	-34.549	24.830	1.00	61.96	A
2822	CA	ALA	A1370	-20.172	-33.416	23.895	1.00	62.59	A
2823	CB	ALA	A1370	-19.118	-32.342	24.336	1.00	63.83	A
2824	C	ALA	A1370	-19.871	-33.976	22.501	1.00	62.10	A
2825	O	ALA	A1370	-18.715	-34.345	22.227	1.00	63.18	A
2826	N	GLY	A1371	-20.892	-34.108	21.648	1.00	60.40	A
2827	CA	GLY	A1371	-20.773	-34.970	20.506	1.00	58.60	A
2828	C	GLY	A1371	-19.939	-34.411	19.456	1.00	58.08	A
2829	O	GLY	A1371	-18.817	-34.773	19.289	1.00	59.80	A
2830	N	ASP	A1372	-20.491	-33.414	18.807	1.00	59.75	A
2831	CA	ASP	A1372	-20.010	-32.835	17.464	1.00	60.25	A
2832	CB	ASP	A1372	-18.870	-33.568	16.645	1.00	58.55	A
2833	CG	ASP	A1372	-18.037	-32.542	15.950	1.00	59.09	A
2834	OD1	ASP	A1372	-16.851	-32.774	15.522	1.00	61.64	A
2835	OD2	ASP	A1372	-18.619	-31.420	15.951	1.00	49.16	A
2836	C	ASP	A1372	-21.195	-32.364	16.542	1.00	57.63	A
2837	O	ASP	A1372	-21.160	-31.270	15.924	1.00	58.29	A
2838	N	SER	A1373	-22.237	-33.134	16.607	1.00	54.78	A
2839	CA	SER	A1373	-23.547	-32.668	16.301	1.00	58.17	A
2840	CB	SER	A1373	-24.329	-33.900	15.662	1.00	58.40	A
2841	OG	SER	A1373	-23.386	-34.754	14.832	1.00	55.35	A
2842	C	SER	A1373	-24.261	-31.992	17.573	1.00	59.57	A
2843	O	SER	A1373	-25.511	-31.881	17.687	1.00	60.06	A

2844	N	GLU	A1374	-23.472	-31.621	18.573	1.00	59.34	A
2845	CA	GLU	A1374	-24.018	-30.731	19.589	1.00	60.82	A
2846	CB	GLU	A1374	-24.154	-31.368	20.982	1.00	61.04	A
2847	CG	GLU	A1374	-25.035	-32.690	20.880	1.00	62.49	A
2848	CD	GLU	A1374	-24.250	-33.999	20.518	1.00	63.95	A
2849	OE1	GLU	A1374	-23.000	-33.972	20.152	1.00	56.36	A
2850	OE2	GLU	A1374	-24.909	-35.084	20.635	1.00	65.88	A
2851	C	GLU	A1374	-23.249	-29.409	19.616	1.00	59.88	A
2852	O	GLU	A1374	-23.724	-28.467	20.214	1.00	62.58	A
2853	N	LEU	A1375	-22.097	-29.325	18.957	1.00	55.89	A
2854	CA	LEU	A1375	-21.377	-28.058	18.794	1.00	50.93	A
2855	CB	LEU	A1375	-20.117	-28.300	17.967	1.00	51.15	A
2856	CG	LEU	A1375	-18.690	-28.543	18.604	1.00	51.01	A
2857	CD1	LEU	A1375	-18.635	-29.075	20.074	1.00	47.34	A
2858	CD2	LEU	A1375	-17.724	-29.339	17.673	1.00	46.16	A
2859	C	LEU	A1375	-22.158	-26.860	18.128	1.00	50.72	A
2860	O	LEU	A1375	-22.624	-27.002	17.007	1.00	48.70	A
2861	N	PHE	A1376	-22.229	-25.692	18.835	1.00	48.72	A
2862	CA	PHE	A1376	-22.783	-24.419	18.340	1.00	48.07	A
2863	CB	PHE	A1376	-23.713	-23.767	19.352	1.00	46.36	A
2864	CG	PHE	A1376	-24.953	-24.535	19.551	1.00	50.49	A
2865	CD1	PHE	A1376	-24.893	-25.837	20.110	1.00	55.68	A
2866	CD2	PHE	A1376	-26.171	-24.031	19.216	1.00	48.27	A
2867	CE1	PHE	A1376	-26.105	-26.620	20.332	1.00	50.46	A
2868	CE2	PHE	A1376	-27.352	-24.775	19.471	1.00	50.20	A
2869	CZ	PHE	A1376	-27.319	-26.070	20.043	1.00	46.59	A
2870	C	PHE	A1376	-21.816	-23.400	18.015	1.00	45.22	A
2871	O	PHE	A1376	-20.937	-23.242	18.810	1.00	49.23	A
2872	N	LEU	A1377	-22.116	-22.605	16.969	1.00	41.02	A
2873	CA	LEU	A1377	-21.401	-21.412	16.571	1.00	37.80	A
2874	CB	LEU	A1377	-21.376	-21.241	15.069	1.00	40.22	A
2875	CG	LEU	A1377	-20.891	-19.863	14.705	1.00	44.81	A
2876	CD1	LEU	A1377	-20.186	-19.903	13.426	1.00	40.72	A
2877	CD2	LEU	A1377	-21.998	-18.551	14.879	1.00	44.75	A
2878	C	LEU	A1377	-22.079	-20.280	17.122	1.00	36.28	A
2879	O	LEU	A1377	-23.177	-20.181	17.036	1.00	36.03	A
2880	N	MET	A1378	-21.454	-19.406	17.818	1.00	38.71	A
2881	CA	MET	A1378	-22.196	-18.340	18.427	1.00	37.60	A
2882	CB	MET	A1378	-22.174	-18.537	19.846	1.00	33.48	A
2883	CG	MET	A1378	-22.623	-17.357	20.556	1.00	39.80	A
2884	SD	MET	A1378	-22.714	-17.585	22.474	1.00	39.02	A
2885	CE	MET	A1378	-21.038	-17.139	22.750	1.00	28.85	A
2886	C	MET	A1378	-21.424	-17.051	17.942	1.00	38.09	A
2887	O	MET	A1378	-20.171	-16.964	17.906	1.00	33.46	A
2888	N	LYS	A1379	-22.255	-16.078	17.548	1.00	40.38	A
2889	CA	LYS	A1379	-21.903	-14.796	16.858	1.00	43.90	A
2890	CB	LYS	A1379	-22.495	-14.813	15.367	1.00	45.91	A
2891	CG	LYS	A1379	-22.918	-13.479	14.672	1.00	41.93	A
2892	CD	LYS	A1379	-22.212	-13.455	13.330	1.00	53.38	A
2893	CE	LYS	A1379	-22.495	-12.291	12.484	1.00	50.65	A
2894	NZ	LYS	A1379	-23.278	-12.935	11.335	1.00	50.59	A
2895	C	LYS	A1379	-22.537	-13.635	17.620	1.00	45.00	A
2896	O	LYS	A1379	-23.868	-13.523	17.759	1.00	44.44	A
2897	N	LEU	A1380	-21.609	-12.826	18.151	1.00	45.05	A
2898	CA	LEU	A1380	-21.993	-11.588	18.936	1.00	44.97	A
2899	CB	LEU	A1380	-20.727	-10.914	19.384	1.00	43.50	A

2900	CG	LEU	A1380	-20.855	-9.992	20.514	1.00	40.79	A
2901	CD1	LEU	A1380	-19.627	-9.272	20.552	1.00	32.67	A
2902	CD2	LEU	A1380	-21.810	-9.113	20.137	1.00	39.10	A
2903	C	LEU	A1380	-22.493	-10.777	17.783	1.00	43.17	A
2904	O	LEU	A1380	-21.780	-10.794	16.816	1.00	43.12	A
2905	N	ILE	A1381	-23.679	-10.179	17.848	1.00	42.15	A
2906	CA	ILE	A1381	-24.169	-9.337	16.739	1.00	42.48	A
2907	CB	ILE	A1381	-25.561	-9.838	16.048	1.00	42.09	A
2908	CG2	ILE	A1381	-25.314	-11.144	15.494	1.00	47.74	A
2909	CG1	ILE	A1381	-26.791	-10.063	16.888	1.00	32.03	A
2910	CD1	ILE	A1381	-27.478	-8.735	17.407	1.00	28.32	A
2911	C	ILE	A1381	-24.378	-7.880	16.905	1.00	42.12	A
2912	O	ILE	A1381	-24.665	-7.196	15.875	1.00	38.08	A
2913	N	ASN	A1382	-24.391	-7.487	18.217	1.00	41.13	A
2914	CA	ASN	A1382	-24.503	-6.135	18.622	1.00	39.52	A
2915	CB	ASN	A1382	-25.546	-6.037	19.687	1.00	39.27	A
2916	CG	ASN	A1382	-25.103	-6.614	21.077	1.00	45.27	A
2917	OD1	ASN	A1382	-24.073	-7.418	21.223	1.00	44.38	A
2918	ND2	ASN	A1382	-25.916	-6.255	22.119	1.00	27.56	A
2919	C	ASN	A1382	-23.276	-5.316	18.985	1.00	39.89	A
2920	O	ASN	A1382	-23.441	-4.268	19.703	1.00	43.98	A
2921	N	ARG	A1383	-22.075	-5.636	18.500	1.00	39.19	A
2922	CA	ARG	A1383	-20.851	-4.809	18.822	1.00	36.86	A
2923	CB	ARG	A1383	-19.963	-5.444	19.881	1.00	35.30	A
2924	CG	ARG	A1383	-20.520	-5.483	21.112	1.00	32.24	A
2925	CD	ARG	A1383	-21.164	-4.022	21.391	1.00	30.14	A
2926	NE	ARG	A1383	-20.967	-3.686	22.762	1.00	33.68	A
2927	CZ	ARG	A1383	-21.820	-3.950	23.768	1.00	36.69	A
2928	NH1	ARG	A1383	-23.121	-4.249	23.468	1.00	29.53	A
2929	NH2	ARG	A1383	-21.467	-3.624	25.082	1.00	34.36	A
2930	C	ARG	A1383	-19.960	-4.640	17.642	1.00	37.80	A
2931	O	ARG	A1383	-18.841	-5.000	17.687	1.00	36.84	A
2932	N	PRO	A1384	-20.482	-4.112	16.528	1.00	39.69	A
2933	CD	PRO	A1384	-21.777	-3.512	16.215	1.00	37.34	A
2934	CA	PRO	A1384	-19.716	-4.266	15.327	1.00	38.56	A
2935	CB	PRO	A1384	-20.763	-4.035	14.328	1.00	34.74	A
2936	CG	PRO	A1384	-21.560	-3.219	14.928	1.00	33.26	A
2937	C	PRO	A1384	-18.672	-3.196	15.424	1.00	41.20	A
2938	O	PRO	A1384	-17.581	-3.263	14.787	1.00	41.75	A
2939	N	ILE	A1385	-19.024	-2.257	16.318	1.00	41.94	A
2940	CA	ILE	A1385	-18.159	-1.118	16.669	1.00	43.36	A
2941	CB	ILE	A1385	-19.073	0.030	16.345	1.00	41.65	A
2942	CG2	ILE	A1385	-19.700	0.447	17.528	1.00	46.55	A
2943	CG1	ILE	A1385	-18.439	1.343	16.001	1.00	47.51	A
2944	CD1	ILE	A1385	-19.625	2.647	16.196	1.00	40.88	A
2945	C	ILE	A1385	-17.944	-1.376	18.280	1.00	42.53	A
2946	O	ILE	A1385	-18.972	-1.439	18.965	1.00	40.52	A
2947	N	ILE	A1386	-16.739	-1.627	18.839	1.00	41.78	A
2948	CA	ILE	A1386	-16.537	-1.995	20.362	1.00	42.59	A
2949	CB	ILE	A1386	-16.050	-3.541	20.709	1.00	45.19	A
2950	CG2	ILE	A1386	-17.013	-4.336	21.980	1.00	40.21	A
2951	CG1	ILE	A1386	-15.779	-4.349	19.441	1.00	41.40	A
2952	CD1	ILE	A1386	-14.726	-3.789	18.775	1.00	45.03	A
2953	C	ILE	A1386	-15.459	-1.177	21.117	1.00	41.86	A
2954	O	ILE	A1386	-14.618	-0.543	20.514	1.00	41.93	A
2955	N	VAL	A1387	-15.427	-1.245	22.441	1.00	42.02	A

2956	CA	VAL	A1387	-14.409	-0.485	23.282	1.00	39.92	A
2957	CB	VAL	A1387	-14.914	0.927	23.623	1.00	40.61	A
2958	CG1	VAL	A1387	-13.816	1.749	24.445	1.00	44.19	A
2959	CG2	VAL	A1387	-15.175	1.640	22.175	1.00	34.79	A
2960	C	VAL	A1387	-14.169	-1.383	24.421	1.00	37.51	A
2961	O	VAL	A1387	-15.115	-1.992	24.795	1.00	37.27	A
2962	N	PHE	A1388	-12.961	-1.532	24.916	1.00	36.60	A
2963	CA	PHE	A1388	-12.661	-2.626	25.950	1.00	38.89	A
2964	CB	PHE	A1388	-11.507	-3.597	25.495	1.00	41.04	A
2965	CG	PHE	A1388	-11.807	-4.344	24.201	1.00	40.99	A
2966	CD1	PHE	A1388	-12.662	-5.475	24.213	1.00	39.56	A
2967	CD2	PHE	A1388	-11.499	-3.728	22.916	1.00	45.41	A
2968	CE1	PHE	A1388	-12.970	-6.214	23.009	1.00	36.39	A
2969	CE2	PHE	A1388	-11.788	-4.421	21.632	1.00	40.60	A
2970	CZ	PHE	A1388	-12.516	-5.701	21.742	1.00	42.12	A
2971	C	PHE	A1388	-12.154	-1.980	27.071	1.00	38.56	A
2972	O	PHE	A1388	-11.235	-1.241	26.953	1.00	44.46	A
2973	N	ARG	A1389	-12.858	-2.030	28.128	1.00	38.79	A
2974	CA	ARG	A1389	-12.418	-1.473	29.428	1.00	38.76	A
2975	CB	ARG	A1389	-13.558	-0.889	30.124	1.00	37.37	A
2976	CG	ARG	A1389	-13.031	0.046	31.281	1.00	39.11	A
2977	CD	ARG	A1389	-14.232	0.265	32.150	1.00	42.37	A
2978	NE	ARG	A1389	-14.315	1.585	32.575	1.00	43.25	A
2979	CZ	ARG	A1389	-15.217	2.031	33.454	1.00	39.73	A
2980	NH1	ARG	A1389	-15.952	1.172	33.990	1.00	35.19	A
2981	NH2	ARG	A1389	-15.327	3.331	33.809	1.00	45.09	A
2982	C	ARG	A1389	-12.022	-2.479	30.456	1.00	40.28	A
2983	O	ARG	A1389	-12.921	-3.213	30.859	1.00	36.19	A
2984	N	GLY	A1390	-10.677	-2.569	30.716	1.00	43.57	A
2985	CA	GLY	A1390	-10.002	-3.327	31.799	1.00	47.33	A
2986	C	GLY	A1390	-10.238	-2.811	33.276	1.00	49.93	A
2987	O	GLY	A1390	-11.285	-2.935	33.794	1.00	50.03	A
2988	N	GLU	A1391	-9.311	-2.157	33.893	1.00	53.45	A
2989	CA	GLU	A1391	-9.013	-2.226	35.398	1.00	56.77	A
2990	CB	GLU	A1391	-7.758	-3.095	35.556	1.00	58.18	A
2991	CG	GLU	A1391	-8.139	-4.533	35.658	1.00	62.62	A
2992	CD	GLU	A1391	-7.448	-5.338	36.855	1.00	64.88	A
2993	OE1	GLU	A1391	-6.168	-5.615	36.842	1.00	60.83	A
2994	OE2	GLU	A1391	-8.253	-5.732	37.767	1.00	58.76	A
2995	C	GLU	A1391	-8.558	-0.830	35.931	1.00	57.24	A
2996	O	GLU	A1391	-9.247	-0.202	36.639	1.00	59.18	A
2997	N	HIS	A1392	-7.369	-0.360	35.525	1.00	57.11	A
2998	CA	HIS	A1392	-7.042	1.066	35.528	1.00	56.66	A
2999	CB	HIS	A1392	-5.745	1.325	36.453	1.00	59.76	A
3000	CG	HIS	A1392	-5.502	0.184	37.406	1.00	63.94	A
3001	CD2	HIS	A1392	-4.603	-0.836	37.324	1.00	65.69	A
3002	ND1	HIS	A1392	-6.432	-0.181	38.388	1.00	57.85	A
3003	CE1	HIS	A1392	-6.106	-1.376	38.840	1.00	62.73	A
3004	NE2	HIS	A1392	-4.952	-1.550	38.243	1.00	63.71	A
3005	C	HIS	A1392	-6.907	1.498	34.023	1.00	55.22	A
3006	O	HIS	A1392	-5.787	1.848	33.583	1.00	54.00	A
3007	N	GLY	A1393	-8.019	1.331	33.244	1.00	52.49	A
3008	CA	GLY	A1393	-8.392	2.092	32.026	1.00	50.24	A
3009	C	GLY	A1393	-8.917	1.420	30.742	1.00	49.56	A
3010	O	GLY	A1393	-9.255	0.198	30.650	1.00	52.43	A
3011	N	PHE	A1394	-8.852	2.131	29.658	1.00	46.49	A

3012	CA	PHE	A1394	-9.414	1.525	28.464	1.00	45.59	A
3013	CB	PHE	A1394	-10.171	2.561	27.601	1.00	43.86	A
3014	CG	PHE	A1394	-11.489	3.014	28.269	1.00	37.61	A
3015	CD1	PHE	A1394	-11.520	4.169	28.958	1.00	27.24	A
3016	CD2	PHE	A1394	-12.623	2.203	28.267	1.00	34.34	A
3017	CE1	PHE	A1394	-12.587	4.590	29.616	1.00	30.36	A
3018	CE2	PHE	A1394	-13.799	2.681	28.810	1.00	35.30	A
3019	CZ	PHE	A1394	-13.801	3.892	29.489	1.00	39.72	A
3020	C	PHE	A1394	-8.420	0.775	27.680	1.00	46.38	A
3021	O	PHE	A1394	-7.190	1.075	27.819	1.00	49.95	A
3022	N	ILE	A1395	-8.879	-0.142	26.834	1.00	44.41	A
3023	CA	ILE	A1395	-7.984	-0.512	25.745	1.00	44.34	A
3024	CB	ILE	A1395	-8.258	-1.849	25.191	1.00	44.43	A
3025	CG2	ILE	A1395	-7.171	-2.287	24.321	1.00	44.81	A
3026	CG1	ILE	A1395	-8.457	-2.964	26.273	1.00	45.92	A
3027	CD1	ILE	A1395	-8.503	-4.542	25.541	1.00	50.31	A
3028	C	ILE	A1395	-7.871	0.564	24.669	1.00	43.95	A
3029	O	ILE	A1395	-8.747	1.324	24.356	1.00	42.42	A
3030	N	GLY	A1396	-6.683	0.648	24.172	1.00	47.46	A
3031	CA	GLY	A1396	-6.192	1.804	23.410	1.00	51.27	A
3032	C	GLY	A1396	-4.799	1.592	22.792	1.00	53.85	A
3033	O	GLY	A1396	-3.893	1.016	23.388	1.00	56.79	A
3034	N	CYS	A1397	-4.598	2.031	21.573	1.00	55.64	A
3035	CA	CYS	A1397	-3.307	1.860	21.017	1.00	57.85	A
3036	CB	CYS	A1397	-3.243	2.153	19.478	1.00	56.69	A
3037	SG	CYS	A1397	-4.889	1.812	18.758	1.00	65.91	A
3038	C	CYS	A1397	-2.562	2.935	21.720	1.00	57.37	A
3039	O	CYS	A1397	-3.050	4.077	22.022	1.00	54.23	A
3040	N	ARG	A1398	-1.328	2.536	21.872	1.00	58.80	A
3041	CA	ARG	A1398	-0.274	3.475	21.743	1.00	59.63	A
3042	CB	ARG	A1398	1.030	2.812	21.483	1.00	58.62	A
3043	CG	ARG	A1398	2.198	3.498	22.273	1.00	62.50	A
3044	CD	ARG	A1398	2.091	3.518	23.780	1.00	65.92	A
3045	NE	ARG	A1398	2.406	2.212	24.346	1.00	68.01	A
3046	CZ	ARG	A1398	2.353	1.874	25.653	1.00	75.31	A
3047	NH1	ARG	A1398	1.998	2.720	26.639	1.00	73.15	A
3048	NH2	ARG	A1398	2.657	0.623	26.019	1.00	81.89	A
3049	C	ARG	A1398	-0.509	4.703	20.838	1.00	60.42	A
3050	O	ARG	A1398	-1.609	5.246	20.702	1.00	58.64	A
3051	N	LYS	A1399	0.611	5.275	20.470	1.00	63.88	A
3052	CA	LYS	A1399	0.690	6.620	19.923	1.00	64.03	A
3053	CB	LYS	A1399	1.254	7.666	20.946	1.00	64.69	A
3054	CG	LYS	A1399	1.305	9.322	20.357	1.00	64.27	A
3055	CD	LYS	A1399	2.509	10.409	20.738	1.00	59.24	A
3056	CE	LYS	A1399	4.076	9.883	20.910	1.00	54.47	A
3057	NZ	LYS	A1399	5.076	11.101	21.302	1.00	60.13	A
3058	C	LYS	A1399	1.530	6.431	18.590	1.00	64.70	A
3059	O	LYS	A1399	0.934	6.332	17.485	1.00	67.48	A
3060	N	VAL	A1400	2.839	6.255	18.679	1.00	62.52	A
3061	CA	VAL	A1400	3.602	5.989	17.536	1.00	61.69	A
3062	CB	VAL	A1400	4.418	7.297	17.125	1.00	64.66	A
3063	CG1	VAL	A1400	4.885	7.315	15.487	1.00	65.86	A
3064	CG2	VAL	A1400	3.634	8.678	17.572	1.00	61.99	A
3065	C	VAL	A1400	4.484	4.776	17.754	1.00	61.76	A
3066	O	VAL	A1400	5.575	4.741	17.205	1.00	62.66	A
3067	N	THR	A1401	4.016	3.778	18.548	1.00	61.99	A

3068	CA	THR	A1401	4.499	2.298	18.521	1.00	59.76	A
3069	CB	THR	A1401	4.969	1.804	20.022	1.00	60.83	A
3070	OG1	THR	A1401	6.462	1.823	20.260	1.00	55.71	A
3071	CG2	THR	A1401	4.230	0.409	20.378	1.00	53.54	A
3072	C	THR	A1401	3.560	1.154	17.849	1.00	59.89	A
3073	O	THR	A1401	3.993	0.159	17.251	1.00	60.51	A
3074	N	GLY	A1402	2.265	1.243	17.980	1.00	57.87	A
3075	CA	GLY	A1402	1.576	0.119	17.576	1.00	57.98	A
3076	C	GLY	A1402	0.889	-0.397	18.796	1.00	57.80	A
3077	O	GLY	A1402	-0.306	-0.702	18.714	1.00	59.21	A
3078	N	THR	A1403	1.592	-0.378	19.942	1.00	57.69	A
3079	CA	THR	A1403	1.298	-1.360	21.048	1.00	53.83	A
3080	CB	THR	A1403	2.400	-1.620	22.101	1.00	52.23	A
3081	OG1	THR	A1403	3.673	-1.786	21.443	1.00	54.49	A
3082	CG2	THR	A1403	2.134	-2.880	22.618	1.00	44.58	A
3083	C	THR	A1403	-0.014	-1.187	21.672	1.00	52.84	A
3084	O	THR	A1403	-0.520	-0.014	21.866	1.00	51.18	A
3085	N	LEU	A1404	-0.637	-2.339	21.859	1.00	51.28	A
3086	CA	LEU	A1404	-1.815	-2.254	22.524	1.00	52.39	A
3087	CB	LEU	A1404	-2.794	-3.330	22.136	1.00	52.14	A
3088	CG	LEU	A1404	-3.644	-3.234	20.813	1.00	46.24	A
3089	CD1	LEU	A1404	-4.237	-1.922	20.423	1.00	42.27	A
3090	CD2	LEU	A1404	-2.953	-3.781	19.614	1.00	47.59	A
3091	C	LEU	A1404	-1.666	-1.915	24.038	1.00	55.39	A
3092	O	LEU	A1404	-0.855	-2.486	24.719	1.00	57.16	A
3093	N	ASP	A1405	-2.341	-0.842	24.502	1.00	57.13	A
3094	CA	ASP	A1405	-2.455	-0.523	25.904	1.00	56.29	A
3095	CB	ASP	A1405	-2.743	0.923	25.986	1.00	57.29	A
3096	CG	ASP	A1405	-1.511	1.693	26.209	1.00	66.43	A
3097	OD1	ASP	A1405	-0.693	1.710	25.225	1.00	77.55	A
3098	OD2	ASP	A1405	-1.309	2.196	27.376	1.00	67.72	A
3099	C	ASP	A1405	-3.555	-1.243	26.704	1.00	55.00	A
3100	O	ASP	A1405	-4.619	-1.506	26.203	1.00	54.88	A
3101	N	ALA	A1406	-3.312	-1.504	27.978	1.00	53.42	A
3102	CA	ALA	A1406	-4.373	-1.965	28.780	1.00	53.18	A
3103	CB	ALA	A1406	-3.923	-3.028	29.642	1.00	51.53	A
3104	C	ALA	A1406	-4.958	-0.888	29.597	1.00	54.00	A
3105	O	ALA	A1406	-5.854	-1.148	30.420	1.00	56.14	A
3106	N	ASN	A1407	-4.453	0.318	29.461	1.00	53.28	A
3107	CA	ASN	A1407	-4.733	1.227	30.523	1.00	53.63	A
3108	CB	ASN	A1407	-3.683	1.020	31.575	1.00	54.49	A
3109	CG	ASN	A1407	-2.374	1.678	31.198	1.00	54.66	A
3110	OD1	ASN	A1407	-2.355	2.742	30.630	1.00	57.87	A
3111	ND2	ASN	A1407	-1.251	1.013	31.506	1.00	55.66	A
3112	C	ASN	A1407	-4.734	2.703	30.169	1.00	54.57	A
3113	O	ASN	A1407	-4.278	3.572	30.979	1.00	53.32	A
3114	N	ARG	A1408	-5.206	3.029	28.975	1.00	54.11	A
3115	CA	ARG	A1408	-4.997	4.372	28.588	1.00	54.32	A
3116	CB	ARG	A1408	-4.973	4.435	27.064	1.00	55.69	A
3117	CG	ARG	A1408	-4.066	3.455	26.442	1.00	53.69	A
3118	CD	ARG	A1408	-3.541	3.857	24.936	1.00	57.92	A
3119	NE	ARG	A1408	-3.167	5.242	24.597	1.00	51.71	A
3120	CZ	ARG	A1408	-4.087	6.079	24.208	1.00	48.26	A
3121	NH1	ARG	A1408	-3.776	7.313	23.920	1.00	38.43	A
3122	NH2	ARG	A1408	-5.324	5.632	24.181	1.00	44.81	A
3123	C	ARG	A1408	-6.202	5.001	29.276	1.00	52.91	A

3124	O	ARG	A1408	-6.972	4.217	29.876	1.00	52.61	A
3125	N	SER	A1409	-6.383	6.328	29.215	1.00	51.70	A
3126	CA	SER	A1409	-7.515	7.066	30.013	1.00	53.20	A
3127	CB	SER	A1409	-6.906	8.303	30.624	1.00	49.62	A
3128	OG	SER	A1409	-6.370	8.882	29.468	1.00	58.82	A
3129	C	SER	A1409	-8.889	7.334	29.204	1.00	50.11	A
3130	O	SER	A1409	-9.942	7.997	29.579	1.00	46.60	A
3131	N	SER	A1410	-8.844	6.733	28.050	1.00	50.98	A
3132	CA	SER	A1410	-9.700	7.194	26.921	1.00	50.18	A
3133	CB	SER	A1410	-9.147	8.432	26.245	1.00	48.65	A
3134	OG	SER	A1410	-9.794	9.550	26.770	1.00	45.04	A
3135	C	SER	A1410	-9.692	6.025	25.953	1.00	50.85	A
3136	O	SER	A1410	-8.574	5.462	25.628	1.00	47.73	A
3137	N	TYR	A1411	-10.957	5.723	25.576	1.00	49.51	A
3138	CA	TYR	A1411	-11.429	4.610	24.850	1.00	47.90	A
3139	CB	TYR	A1411	-12.806	4.303	25.388	1.00	46.95	A
3140	CG	TYR	A1411	-13.804	5.541	25.462	1.00	49.28	A
3141	CD1	TYR	A1411	-14.183	6.311	24.319	1.00	47.47	A
3142	CE1	TYR	A1411	-15.056	7.322	24.447	1.00	52.92	A
3143	CD2	TYR	A1411	-14.448	5.823	26.637	1.00	47.69	A
3144	CE2	TYR	A1411	-15.342	6.906	26.823	1.00	44.51	A
3145	CZ	TYR	A1411	-15.656	7.684	25.770	1.00	51.14	A
3146	OH	TYR	A1411	-16.713	8.687	25.945	1.00	38.52	A
3147	C	TYR	A1411	-11.507	4.853	23.363	1.00	48.38	A
3148	O	TYR	A1411	-12.553	5.266	22.796	1.00	51.63	A
3149	N	ASP	A1412	-10.424	4.536	22.704	1.00	47.64	A
3150	CA	ASP	A1412	-10.428	4.020	21.295	1.00	46.55	A
3151	CB	ASP	A1412	-9.089	3.408	21.065	1.00	49.73	A
3152	CG	ASP	A1412	-7.980	4.463	20.986	1.00	51.41	A
3153	OD1	ASP	A1412	-7.187	4.317	20.092	1.00	60.54	A
3154	OD2	ASP	A1412	-7.846	5.404	21.773	1.00	54.02	A
3155	C	ASP	A1412	-11.511	3.103	20.769	1.00	46.25	A
3156	O	ASP	A1412	-11.814	2.069	21.358	1.00	49.69	A
3157	N	VAL	A1413	-12.184	3.501	19.691	1.00	45.90	A
3158	CA	VAL	A1413	-13.340	2.677	19.034	1.00	42.01	A
3159	CB	VAL	A1413	-14.464	3.497	18.458	1.00	37.35	A
3160	CG1	VAL	A1413	-15.666	2.859	18.616	1.00	31.40	A
3161	CG2	VAL	A1413	-14.658	4.645	19.266	1.00	35.27	A
3162	C	VAL	A1413	-12.776	1.780	17.950	1.00	44.36	A
3163	O	VAL	A1413	-11.957	2.271	17.045	1.00	45.80	A
3164	N	PHE	A1414	-13.031	0.468	18.178	1.00	45.45	A
3165	CA	PHE	A1414	-12.605	-0.611	17.298	1.00	46.30	A
3166	CB	PHE	A1414	-11.938	-1.792	18.033	1.00	42.88	A
3167	CG	PHE	A1414	-10.616	-1.461	18.507	1.00	44.57	A
3168	CD1	PHE	A1414	-9.661	-1.101	17.553	1.00	41.91	A
3169	CD2	PHE	A1414	-10.286	-1.359	19.959	1.00	32.91	A
3170	CE1	PHE	A1414	-8.379	-0.649	18.015	1.00	44.10	A
3171	CE2	PHE	A1414	-8.949	-0.945	20.354	1.00	35.71	A
3172	CZ	PHE	A1414	-8.039	-0.583	19.417	1.00	37.20	A
3173	C	PHE	A1414	-13.780	-1.137	16.530	1.00	48.20	A
3174	O	PHE	A1414	-14.890	-1.224	17.099	1.00	49.41	A
3175	N	GLN	A1415	-13.498	-1.605	15.312	1.00	47.55	A
3176	CA	GLN	A1415	-14.416	-2.542	14.767	1.00	49.28	A
3177	CB	GLN	A1415	-15.020	-1.875	13.493	1.00	50.13	A
3178	CG	GLN	A1415	-14.114	-1.864	12.284	1.00	53.96	A
3179	CD	GLN	A1415	-14.031	-0.483	11.626	1.00	54.78	A

3180	OE1	GLN	A1415	-12.961	0.099	11.665	1.00	55.88	A
3181	NE2	GLN	A1415	-15.143	0.041	11.036	1.00	43.53	A
3182	C	GLN	A1415	-14.120	-4.150	14.778	1.00	48.22	A
3183	O	GLN	A1415	-13.046	-4.614	15.070	1.00	45.53	A
3184	N	LEU	A1416	-15.085	-4.990	14.422	1.00	48.46	A
3185	CA	LEU	A1416	-15.006	-6.358	14.814	1.00	48.37	A
3186	CB	LEU	A1416	-15.746	-6.410	16.145	1.00	49.02	A
3187	CG	LEU	A1416	-16.466	-7.317	17.109	1.00	49.16	A
3188	CD1	LEU	A1416	-17.299	-8.263	16.356	1.00	58.06	A
3189	CD2	LEU	A1416	-15.314	-7.977	17.719	1.00	53.63	A
3190	C	LEU	A1416	-15.780	-7.073	13.757	1.00	49.15	A
3191	O	LEU	A1416	-16.932	-6.889	13.665	1.00	48.25	A
3192	N	GLU	A1417	-15.089	-7.830	12.904	1.00	50.70	A
3193	CA	GLU	A1417	-15.752	-8.747	11.982	1.00	48.83	A
3194	CB	GLU	A1417	-15.107	-8.857	10.563	1.00	47.46	A
3195	CG	GLU	A1417	-13.766	-8.649	10.361	1.00	47.67	A
3196	CD	GLU	A1417	-13.467	-7.377	9.548	1.00	48.25	A
3197	OE1	GLU	A1417	-12.506	-7.335	8.740	1.00	47.35	A
3198	OE2	GLU	A1417	-14.072	-6.345	9.760	1.00	43.04	A
3199	C	GLU	A1417	-15.831	-10.078	12.436	1.00	48.09	A
3200	O	GLU	A1417	-14.888	-10.605	12.737	1.00	50.19	A
3201	N	PHE	A1418	-16.957	-10.724	12.229	1.00	50.97	A
3202	CA	PHE	A1418	-17.060	-12.120	12.522	1.00	51.40	A
3203	CB	PHE	A1418	-18.446	-12.513	12.676	1.00	48.90	A
3204	CG	PHE	A1418	-18.557	-13.812	13.454	1.00	54.09	A
3205	CD1	PHE	A1418	-17.898	-13.944	14.738	1.00	51.99	A
3206	CD2	PHE	A1418	-19.286	-14.851	12.992	1.00	52.06	A
3207	CE1	PHE	A1418	-18.007	-15.061	15.467	1.00	49.04	A
3208	CE2	PHE	A1418	-19.412	-16.074	13.814	1.00	55.11	A
3209	CZ	PHE	A1418	-18.748	-16.203	14.971	1.00	47.77	A
3210	C	PHE	A1418	-16.612	-13.105	11.498	1.00	53.47	A
3211	O	PHE	A1418	-16.803	-12.919	10.292	1.00	54.29	A
3212	N	ASN	A1419	-16.246	-14.287	12.001	1.00	55.96	A
3213	CA	ASN	A1419	-15.714	-15.351	11.129	1.00	54.97	A
3214	CB	ASN	A1419	-14.426	-14.803	10.625	1.00	53.96	A
3215	CG	ASN	A1419	-13.768	-15.671	9.639	1.00	58.56	A
3216	OD1	ASN	A1419	-14.368	-16.204	8.686	1.00	61.83	A
3217	ND2	ASN	A1419	-12.472	-15.756	9.801	1.00	60.97	A
3218	C	ASN	A1419	-15.563	-16.740	11.776	1.00	53.54	A
3219	O	ASN	A1419	-14.483	-17.081	12.214	1.00	53.40	A
3220	N	ASP	A1420	-16.703	-17.492	11.883	1.00	51.85	A
3221	CA	ASP	A1420	-16.686	-18.944	12.143	1.00	49.02	A
3222	CB	ASP	A1420	-15.592	-19.623	11.195	1.00	49.36	A
3223	CG	ASP	A1420	-15.494	-21.171	11.355	1.00	49.16	A
3224	OD1	ASP	A1420	-16.414	-21.862	11.845	1.00	42.25	A
3225	OD2	ASP	A1420	-14.470	-21.727	10.994	1.00	52.11	A
3226	C	ASP	A1420	-16.240	-19.058	13.543	1.00	47.72	A
3227	O	ASP	A1420	-15.102	-19.468	13.746	1.00	50.48	A
3228	N	GLY	A1421	-17.045	-18.660	14.523	1.00	45.62	A
3229	CA	GLY	A1421	-16.549	-18.651	15.947	1.00	43.81	A
3230	C	GLY	A1421	-15.367	-17.804	16.431	1.00	42.51	A
3231	O	GLY	A1421	-15.296	-17.544	17.582	1.00	42.31	A
3232	N	ALA	A1422	-14.450	-17.407	15.512	1.00	43.57	A
3233	CA	ALA	A1422	-13.479	-16.273	15.661	1.00	43.56	A
3234	CB	ALA	A1422	-12.304	-16.575	14.829	1.00	44.75	A
3235	C	ALA	A1422	-13.864	-14.732	15.525	1.00	40.33	A

3236	O	ALA	A1422	-14.949	-14.469	15.200	1.00	41.87	A
3237	N	TYR	A1423	-12.995	-13.801	15.855	1.00	35.32	A
3238	CA	TYR	A1423	-13.331	-12.422	15.981	1.00	39.01	A
3239	CB	TYR	A1423	-13.610	-11.833	17.469	1.00	39.45	A
3240	CG	TYR	A1423	-14.991	-12.217	17.977	1.00	41.46	A
3241	CD1	TYR	A1423	-15.219	-13.483	18.665	1.00	38.54	A
3242	CE1	TYR	A1423	-16.448	-13.870	19.055	1.00	28.82	A
3243	CD2	TYR	A1423	-16.119	-11.491	17.562	1.00	37.92	A
3244	CE2	TYR	A1423	-17.404	-11.962	17.897	1.00	39.03	A
3245	CZ	TYR	A1423	-17.572	-13.143	18.669	1.00	37.94	A
3246	OH	TYR	A1423	-18.942	-13.554	19.019	1.00	40.40	A
3247	C	TYR	A1423	-12.028	-11.926	15.566	1.00	41.82	A
3248	O	TYR	A1423	-11.009	-12.574	15.795	1.00	40.25	A
3249	N	ASN	A1424	-12.057	-10.770	14.924	1.00	44.16	A
3250	CA	ASN	A1424	-10.854	-10.047	14.459	1.00	43.83	A
3251	CB	ASN	A1424	-10.756	-10.119	12.971	1.00	43.72	A
3252	CG	ASN	A1424	-10.584	-11.448	12.482	1.00	48.44	A
3253	OD1	ASN	A1424	-11.502	-12.177	12.329	1.00	44.59	A
3254	ND2	ASN	A1424	-9.339	-11.766	12.124	1.00	61.24	A
3255	C	ASN	A1424	-11.225	-8.549	14.791	1.00	43.02	A
3256	O	ASN	A1424	-12.504	-8.116	14.705	1.00	39.62	A
3257	N	ILE	A1425	-10.203	-7.780	15.125	1.00	38.73	A
3258	CA	ILE	A1425	-10.619	-6.569	15.755	1.00	40.72	A
3259	CB	ILE	A1425	-9.997	-6.345	17.209	1.00	40.76	A
3260	CG2	ILE	A1425	-10.446	-5.052	17.595	1.00	40.31	A
3261	CG1	ILE	A1425	-10.571	-7.368	18.237	1.00	36.71	A
3262	CD1	ILE	A1425	-9.915	-8.524	18.312	1.00	28.51	A
3263	C	ILE	A1425	-9.995	-5.630	14.845	1.00	40.80	A
3264	O	ILE	A1425	-8.990	-5.964	14.476	1.00	42.68	A
3265	N	LYS	A1426	-10.504	-4.486	14.470	1.00	40.71	A
3266	CA	LYS	A1426	-9.836	-3.860	13.386	1.00	42.64	A
3267	CB	LYS	A1426	-10.517	-4.136	12.001	1.00	42.04	A
3268	CG	LYS	A1426	-9.880	-3.541	10.769	1.00	39.40	A
3269	CD	LYS	A1426	-10.773	-3.661	9.550	1.00	41.88	A
3270	CE	LYS	A1426	-9.789	-4.282	8.261	1.00	53.13	A
3271	NZ	LYS	A1426	-10.336	-4.322	6.784	1.00	40.24	A
3272	C	LYS	A1426	-10.042	-2.527	13.940	1.00	46.68	A
3273	O	LYS	A1426	-11.039	-2.233	14.598	1.00	48.57	A
3274	N	ASP	A1427	-9.025	-1.720	13.785	1.00	49.22	A
3275	CA	ASP	A1427	-9.082	-0.396	14.296	1.00	51.18	A
3276	CB	ASP	A1427	-7.685	-0.024	14.728	1.00	49.73	A
3277	CG	ASP	A1427	-6.794	0.320	13.539	1.00	55.99	A
3278	OD1	ASP	A1427	-7.293	0.255	12.304	1.00	52.50	A
3279	OD2	ASP	A1427	-5.589	0.679	13.878	1.00	58.73	A
3280	C	ASP	A1427	-9.638	0.538	13.175	1.00	50.89	A
3281	O	ASP	A1427	-10.440	0.103	12.325	1.00	52.56	A
3282	N	SER	A1428	-9.071	1.723	13.109	1.00	49.65	A
3283	CA	SER	A1428	-9.679	2.852	12.525	1.00	52.00	A
3284	CB	SER	A1428	-9.644	3.951	13.648	1.00	52.54	A
3285	OG	SER	A1428	-10.292	3.312	14.856	1.00	51.14	A
3286	C	SER	A1428	-9.073	3.182	11.125	1.00	53.34	A
3287	O	SER	A1428	-9.794	3.506	10.213	1.00	53.35	A
3288	N	THR	A1429	-7.737	3.056	10.967	1.00	54.86	A
3289	CA	THR	A1429	-7.022	3.169	9.725	1.00	55.03	A
3290	CB	THR	A1429	-5.550	3.276	10.086	1.00	56.05	A
3291	OG1	THR	A1429	-4.960	1.975	10.172	1.00	65.20	A

3292	CG2	THR	A1429	-5.340	3.775	11.475	1.00	53.66	A
3293	C	THR	A1429	-7.309	1.821	8.944	1.00	55.45	A
3294	O	THR	A1429	-7.377	1.776	7.684	1.00	55.57	A
3295	N	GLY	A1430	-7.445	0.721	9.706	1.00	54.68	A
3296	CA	GLY	A1430	-8.210	-0.392	9.290	1.00	52.85	A
3297	C	GLY	A1430	-7.187	-1.495	9.348	1.00	54.24	A
3298	O	GLY	A1430	-7.281	-2.564	8.652	1.00	56.05	A
3299	N	LYS	A1431	-6.219	-1.348	10.233	1.00	53.34	A
3300	CA	LYS	A1431	-5.441	-2.549	10.489	1.00	51.71	A
3301	CB	LYS	A1431	-3.944	-2.342	10.510	1.00	51.45	A
3302	CG	LYS	A1431	-3.327	-1.005	9.796	1.00	57.45	A
3303	CD	LYS	A1431	-2.980	-1.064	8.089	1.00	58.40	A
3304	CE	LYS	A1431	-2.460	0.355	7.487	1.00	43.62	A
3305	NZ	LYS	A1431	-1.498	0.863	8.618	1.00	38.84	A
3306	C	LYS	A1431	-6.069	-3.380	11.614	1.00	51.47	A
3307	O	LYS	A1431	-7.201	-3.124	11.948	1.00	53.10	A
3308	N	TYR	A1432	-5.425	-4.459	12.062	1.00	50.18	A
3309	CA	TYR	A1432	-6.044	-5.664	12.549	1.00	48.23	A
3310	CB	TYR	A1432	-5.789	-6.794	11.578	1.00	47.66	A
3311	CG	TYR	A1432	-6.997	-6.994	10.651	1.00	46.37	A
3312	CD1	TYR	A1432	-8.266	-7.252	11.138	1.00	32.93	A
3313	CE1	TYR	A1432	-9.282	-7.328	10.365	1.00	38.32	A
3314	CD2	TYR	A1432	-6.851	-6.897	9.287	1.00	48.07	A
3315	CE2	TYR	A1432	-7.951	-6.969	8.436	1.00	43.74	A
3316	CZ	TYR	A1432	-9.170	-7.101	8.954	1.00	43.55	A
3317	OH	TYR	A1432	-10.230	-7.152	8.023	1.00	43.02	A
3318	C	TYR	A1432	-5.234	-5.898	13.790	1.00	51.50	A
3319	O	TYR	A1432	-4.035	-5.458	13.792	1.00	53.44	A
3320	N	TRP	A1433	-5.804	-6.499	14.877	1.00	50.76	A
3321	CA	TRP	A1433	-4.994	-6.864	16.093	1.00	48.32	A
3322	CB	TRP	A1433	-5.896	-7.282	17.210	1.00	44.96	A
3323	CG	TRP	A1433	-6.383	-6.126	18.055	1.00	45.32	A
3324	CD2	TRP	A1433	-6.938	-6.144	19.416	1.00	43.18	A
3325	CE2	TRP	A1433	-7.239	-4.828	19.733	1.00	42.41	A
3326	CE3	TRP	A1433	-7.149	-7.150	20.401	1.00	33.86	A
3327	CD1	TRP	A1433	-6.304	-4.854	17.721	1.00	42.54	A
3328	NE1	TRP	A1433	-6.854	-4.080	18.670	1.00	40.10	A
3329	CZ2	TRP	A1433	-7.790	-4.453	20.965	1.00	38.29	A
3330	CZ3	TRP	A1433	-7.782	-6.822	21.446	1.00	38.33	A
3331	CH2	TRP	A1433	-8.060	-5.464	21.780	1.00	40.83	A
3332	C	TRP	A1433	-4.071	-8.063	15.901	1.00	50.43	A
3333	O	TRP	A1433	-4.605	-9.174	15.729	1.00	49.13	A
3334	N	THR	A1434	-2.723	-7.908	15.990	1.00	51.71	A
3335	CA	THR	A1434	-1.883	-9.141	16.024	1.00	51.05	A
3336	CB	THR	A1434	-0.774	-9.105	15.092	1.00	50.46	A
3337	OG1	THR	A1434	-0.454	-7.738	14.904	1.00	48.07	A
3338	CG2	THR	A1434	-1.235	-9.854	13.746	1.00	47.58	A
3339	C	THR	A1434	-1.314	-9.522	17.312	1.00	52.82	A
3340	O	THR	A1434	-1.373	-8.752	18.253	1.00	54.18	A
3341	N	VAL	A1435	-0.719	-10.723	17.374	1.00	54.08	A
3342	CA	VAL	A1435	0.134	-11.010	18.537	1.00	54.41	A
3343	CB	VAL	A1435	-0.277	-12.128	19.474	1.00	54.20	A
3344	CG1	VAL	A1435	0.733	-13.135	19.662	1.00	48.55	A
3345	CG2	VAL	A1435	-0.645	-11.540	20.824	1.00	57.15	A
3346	C	VAL	A1435	1.493	-11.125	18.151	1.00	56.81	A
3347	O	VAL	A1435	1.848	-11.581	17.024	1.00	58.07	A

3348	N	GLY	A1436	2.288	-10.585	19.067	1.00	59.25	A
3349	CA	GLY	A1436	3.758	-10.626	18.907	1.00	59.56	A
3350	C	GLY	A1436	4.490	-11.886	19.374	1.00	58.27	A
3351	O	GLY	A1436	4.090	-12.494	20.416	1.00	58.45	A
3352	N	SER	A1437	5.637	-12.192	18.743	1.00	56.72	A
3353	CA	SER	A1437	6.467	-13.301	19.269	1.00	55.51	A
3354	CB	SER	A1437	7.664	-13.435	18.450	1.00	53.21	A
3355	OG	SER	A1437	8.409	-12.278	18.517	1.00	45.93	A
3356	C	SER	A1437	6.793	-13.248	20.796	1.00	57.44	A
3357	O	SER	A1437	7.064	-14.342	21.469	1.00	58.93	A
3358	N	ASP	A1438	6.725	-12.061	21.422	1.00	57.22	A
3359	CA	ASP	A1438	6.879	-12.056	22.959	1.00	58.69	A
3360	CB	ASP	A1438	7.329	-10.745	23.309	1.00	56.82	A
3361	CG	ASP	A1438	6.683	-9.839	22.430	1.00	57.61	A
3362	OD1	ASP	A1438	5.537	-10.191	21.991	1.00	57.05	A
3363	OD2	ASP	A1438	7.300	-8.864	22.080	1.00	59.56	A
3364	C	ASP	A1438	5.482	-12.204	23.558	1.00	59.84	A
3365	O	ASP	A1438	5.349	-12.212	24.789	1.00	61.61	A
3366	N	SER	A1439	4.468	-12.313	22.681	1.00	60.20	A
3367	CA	SER	A1439	3.040	-12.312	23.096	1.00	62.16	A
3368	CB	SER	A1439	2.770	-13.162	24.340	1.00	62.58	A
3369	OG	SER	A1439	3.255	-14.504	24.307	1.00	65.35	A
3370	C	SER	A1439	2.440	-10.910	23.383	1.00	61.86	A
3371	O	SER	A1439	1.275	-10.770	23.716	1.00	63.05	A
3372	N	ALA	A1440	3.235	-9.863	23.280	1.00	61.29	A
3373	CA	ALA	A1440	2.668	-8.503	23.241	1.00	58.54	A
3374	CB	ALA	A1440	3.775	-7.512	23.328	1.00	56.88	A
3375	C	ALA	A1440	1.916	-8.364	21.916	1.00	56.32	A
3376	O	ALA	A1440	2.481	-8.688	20.817	1.00	53.07	A
3377	N	VAL	A1441	0.641	-7.926	22.074	1.00	55.21	A
3378	CA	VAL	A1441	-0.295	-7.648	20.945	1.00	53.25	A
3379	CB	VAL	A1441	-1.734	-7.595	21.372	1.00	54.21	A
3380	CG1	VAL	A1441	-2.571	-8.182	20.398	1.00	51.72	A
3381	CG2	VAL	A1441	-1.940	-8.353	22.696	1.00	56.26	A
3382	C	VAL	A1441	0.122	-6.328	20.350	1.00	52.19	A
3383	O	VAL	A1441	1.250	-5.876	20.536	1.00	53.25	A
3384	N	THR	A1442	-0.720	-5.820	19.479	1.00	50.61	A
3385	CA	THR	A1442	-0.357	-4.847	18.429	1.00	48.21	A
3386	CB	THR	A1442	0.987	-5.030	17.848	1.00	46.18	A
3387	OG1	THR	A1442	0.915	-4.510	16.528	1.00	48.96	A
3388	CG2	THR	A1442	1.426	-6.401	17.805	1.00	48.07	A
3389	C	THR	A1442	-1.305	-4.652	17.277	1.00	48.20	A
3390	O	THR	A1442	-1.713	-5.537	16.595	1.00	49.92	A
3391	N	SER	A1443	-1.578	-3.426	17.011	1.00	52.16	A
3392	CA	SER	A1443	-2.503	-3.049	16.007	1.00	55.59	A
3393	CB	SER	A1443	-3.056	-1.695	16.333	1.00	56.01	A
3394	OG	SER	A1443	-4.484	-1.701	16.466	1.00	57.45	A
3395	C	SER	A1443	-1.821	-2.931	14.700	1.00	58.69	A
3396	O	SER	A1443	-2.496	-2.759	13.728	1.00	60.44	A
3397	N	SER	A1444	-0.490	-3.053	14.669	1.00	61.51	A
3398	CA	SER	A1444	0.274	-2.790	13.439	1.00	63.92	A
3399	CB	SER	A1444	1.697	-2.336	13.761	1.00	63.64	A
3400	OG	SER	A1444	2.325	-3.070	14.858	1.00	67.87	A
3401	C	SER	A1444	0.270	-3.974	12.540	1.00	66.24	A
3402	O	SER	A1444	0.491	-5.143	13.051	1.00	66.86	A
3403	N	GLY	A1445	0.002	-3.707	11.226	1.00	66.92	A

3404	CA	GLY	A1445	-0.096	-4.814	10.113	1.00	65.00	A
3405	C	GLY	A1445	-1.454	-5.267	9.452	1.00	64.31	A
3406	O	GLY	A1445	-2.528	-4.974	9.969	1.00	62.56	A
3407	N	ASP	A1446	-1.392	-5.975	8.308	1.00	63.66	A
3408	CA	ASP	A1446	-2.624	-6.436	7.559	1.00	63.58	A
3409	CB	ASP	A1446	-2.557	-5.905	6.131	1.00	63.90	A
3410	CG	ASP	A1446	-1.407	-4.913	5.939	1.00	62.61	A
3411	OD1	ASP	A1446	-1.599	-3.684	6.232	1.00	63.62	A
3412	OD2	ASP	A1446	-0.320	-5.370	5.511	1.00	55.74	A
3413	C	ASP	A1446	-2.995	-7.981	7.530	1.00	63.07	A
3414	O	ASP	A1446	-3.763	-8.418	6.671	1.00	61.35	A
3415	N	THR	A1447	-2.474	-8.744	8.517	1.00	63.89	A
3416	CA	THR	A1447	-2.700	-10.187	8.736	1.00	64.88	A
3417	CB	THR	A1447	-1.431	-10.926	9.494	1.00	65.58	A
3418	OG1	THR	A1447	-0.130	-10.392	9.067	1.00	69.94	A
3419	CG2	THR	A1447	-1.400	-12.455	9.321	1.00	60.83	A
3420	C	THR	A1447	-3.905	-10.365	9.670	1.00	66.10	A
3421	O	THR	A1447	-3.642	-10.367	10.897	1.00	66.05	A
3422	N	PRO	A1448	-5.197	-10.622	9.111	1.00	65.93	A
3423	CD	PRO	A1448	-5.680	-10.785	7.706	1.00	66.30	A
3424	CA	PRO	A1448	-6.324	-10.868	10.036	1.00	64.70	A
3425	CB	PRO	A1448	-7.579	-10.853	9.124	1.00	64.81	A
3426	CG	PRO	A1448	-7.133	-10.379	7.744	1.00	65.42	A
3427	C	PRO	A1448	-6.193	-12.137	10.984	1.00	62.51	A
3428	O	PRO	A1448	-6.207	-13.241	10.520	1.00	60.82	A
3429	N	VAL	A1449	-6.125	-11.873	12.324	1.00	60.10	A
3430	CA	VAL	A1449	-5.858	-12.872	13.317	1.00	54.97	A
3431	CB	VAL	A1449	-4.580	-12.657	14.064	1.00	55.21	A
3432	CG1	VAL	A1449	-3.703	-11.655	13.327	1.00	52.90	A
3433	CG2	VAL	A1449	-4.818	-12.429	15.625	1.00	48.82	A
3434	C	VAL	A1449	-6.988	-13.101	14.250	1.00	53.59	A
3435	O	VAL	A1449	-7.364	-12.125	14.977	1.00	54.14	A
3436	N	ASP	A1450	-7.463	-14.381	14.239	1.00	48.44	A
3437	CA	ASP	A1450	-8.496	-14.913	15.077	1.00	46.93	A
3438	CB	ASP	A1450	-8.636	-16.323	14.627	1.00	47.49	A
3439	CG	ASP	A1450	-9.103	-16.478	13.131	1.00	47.44	A
3440	OD1	ASP	A1450	-9.361	-17.589	12.620	1.00	46.11	A
3441	OD2	ASP	A1450	-9.209	-15.513	12.398	1.00	54.11	A
3442	C	ASP	A1450	-8.359	-14.861	16.717	1.00	47.92	A
3443	O	ASP	A1450	-7.398	-15.369	17.357	1.00	45.54	A
3444	N	PHE	A1451	-9.377	-14.277	17.367	1.00	48.96	A
3445	CA	PHE	A1451	-9.526	-14.120	18.800	1.00	46.36	A
3446	CB	PHE	A1451	-9.532	-12.661	19.140	1.00	45.53	A
3447	CG	PHE	A1451	-8.203	-12.035	19.061	1.00	46.73	A
3448	CD1	PHE	A1451	-7.686	-11.614	17.855	1.00	49.62	A
3449	CD2	PHE	A1451	-7.431	-11.860	20.190	1.00	47.90	A
3450	CE1	PHE	A1451	-6.393	-10.946	17.778	1.00	47.91	A
3451	CE2	PHE	A1451	-6.112	-11.213	20.136	1.00	48.89	A
3452	CZ	PHE	A1451	-5.623	-10.737	18.928	1.00	41.41	A
3453	C	PHE	A1451	-10.788	-14.750	19.350	1.00	46.07	A
3454	O	PHE	A1451	-11.675	-15.109	18.645	1.00	47.20	A
3455	N	PHE	A1452	-10.865	-14.909	20.664	1.00	48.03	A
3456	CA	PHE	A1452	-11.949	-15.699	21.296	1.00	47.95	A
3457	CB	PHE	A1452	-11.395	-17.055	21.630	1.00	49.91	A
3458	CG	PHE	A1452	-11.043	-17.834	20.440	1.00	50.45	A
3459	CD1	PHE	A1452	-9.737	-17.889	19.990	1.00	55.15	A

3460	CD2	PHE	A1452	-11.991	-18.431	19.717	1.00	50.68	A
3461	CE1	PHE	A1452	-9.372	-18.634	18.807	1.00	53.49	A
3462	CE2	PHE	A1452	-11.634	-19.178	18.498	1.00	51.86	A
3463	CZ	PHE	A1452	-10.329	-19.243	18.068	1.00	54.24	A
3464	C	PHE	A1452	-12.488	-15.068	22.518	1.00	48.10	A
3465	O	PHE	A1452	-11.790	-14.839	23.488	1.00	50.76	A
3466	N	PHE	A1453	-13.731	-14.696	22.443	1.00	47.79	A
3467	CA	PHE	A1453	-14.347	-13.977	23.503	1.00	48.41	A
3468	CB	PHE	A1453	-15.414	-13.061	22.954	1.00	45.25	A
3469	CG	PHE	A1453	-14.872	-11.860	22.132	1.00	44.75	A
3470	CD1	PHE	A1453	-13.640	-11.824	21.675	1.00	34.91	A
3471	CD2	PHE	A1453	-15.714	-10.771	21.798	1.00	42.03	A
3472	CE1	PHE	A1453	-13.257	-10.816	20.838	1.00	39.14	A
3473	CE2	PHE	A1453	-15.330	-9.676	21.024	1.00	38.07	A
3474	CZ	PHE	A1453	-14.092	-9.670	20.550	1.00	40.58	A
3475	C	PHE	A1453	-15.002	-15.044	24.387	1.00	49.21	A
3476	O	PHE	A1453	-15.859	-15.812	23.972	1.00	50.79	A
3477	N	GLU	A1454	-14.626	-15.119	25.631	1.00	49.46	A
3478	CA	GLU	A1454	-15.357	-16.071	26.393	1.00	49.00	A
3479	CB	GLU	A1454	-14.331	-16.941	27.180	1.00	47.68	A
3480	CG	GLU	A1454	-13.467	-17.792	26.247	1.00	51.72	A
3481	CD	GLU	A1454	-12.579	-18.795	26.914	1.00	53.71	A
3482	OE1	GLU	A1454	-12.019	-19.751	26.172	1.00	55.27	A
3483	OE2	GLU	A1454	-12.491	-18.572	28.134	1.00	47.57	A
3484	C	GLU	A1454	-16.111	-15.097	27.220	1.00	47.50	A
3485	O	GLU	A1454	-15.500	-14.412	27.970	1.00	45.84	A
3486	N	PHE	A1455	-17.406	-14.974	27.076	1.00	47.03	A
3487	CA	PHE	A1455	-18.071	-14.134	28.071	1.00	49.03	A
3488	CB	PHE	A1455	-19.565	-13.711	27.645	1.00	49.34	A
3489	CG	PHE	A1455	-19.586	-13.155	26.319	1.00	41.03	A
3490	CD1	PHE	A1455	-19.315	-13.978	25.273	1.00	34.96	A
3491	CD2	PHE	A1455	-19.687	-11.824	26.150	1.00	41.19	A
3492	CE1	PHE	A1455	-19.278	-13.546	24.074	1.00	31.99	A
3493	CE2	PHE	A1455	-19.534	-11.280	24.886	1.00	37.99	A
3494	CZ	PHE	A1455	-19.318	-12.204	23.829	1.00	40.69	A
3495	C	PHE	A1455	-18.087	-14.785	29.445	1.00	49.24	A
3496	O	PHE	A1455	-19.020	-15.600	29.734	1.00	49.10	A
3497	N	CYS	A1456	-17.063	-14.468	30.232	1.00	49.73	A
3498	CA	CYS	A1456	-16.827	-15.035	31.594	1.00	53.02	A
3499	CB	CYS	A1456	-15.500	-14.609	31.970	1.00	53.38	A
3500	SG	CYS	A1456	-14.506	-15.246	30.680	1.00	66.34	A
3501	C	CYS	A1456	-17.681	-14.453	32.705	1.00	53.38	A
3502	O	CYS	A1456	-18.091	-15.208	33.582	1.00	54.77	A
3503	N	ASP	A1457	-17.910	-13.101	32.667	1.00	52.87	A
3504	CA	ASP	A1457	-18.918	-12.357	33.465	1.00	50.10	A
3505	CB	ASP	A1457	-18.345	-11.161	34.156	1.00	50.96	A
3506	CG	ASP	A1457	-19.022	-10.876	35.482	1.00	49.17	A
3507	OD1	ASP	A1457	-20.198	-11.346	35.663	1.00	51.38	A
3508	OD2	ASP	A1457	-18.377	-10.173	36.318	1.00	48.04	A
3509	C	ASP	A1457	-20.107	-11.839	32.700	1.00	48.82	A
3510	O	ASP	A1457	-20.280	-12.103	31.525	1.00	50.55	A
3511	N	TYR	A1458	-20.904	-11.053	33.406	1.00	47.83	A
3512	CA	TYR	A1458	-22.208	-10.677	33.059	1.00	46.54	A
3513	CB	TYR	A1458	-22.937	-10.545	34.368	1.00	48.79	A
3514	CG	TYR	A1458	-22.764	-9.203	35.055	1.00	49.61	A
3515	CD1	TYR	A1458	-23.865	-8.453	35.361	1.00	45.46	A

3516	CE1	TYR	A1458	-23.747	-7.214	35.897	1.00	55.73	A
3517	CD2	TYR	A1458	-21.475	-8.687	35.348	1.00	54.47	A
3518	CE2	TYR	A1458	-21.317	-7.430	35.938	1.00	58.42	A
3519	CZ	TYR	A1458	-22.468	-6.702	36.216	1.00	58.67	A
3520	OH	TYR	A1458	-22.403	-5.413	36.773	1.00	59.14	A
3521	C	TYR	A1458	-22.246	-9.331	32.376	1.00	48.12	A
3522	O	TYR	A1458	-23.308	-8.793	32.265	1.00	51.05	A
3523	N	ASN	A1459	-21.097	-8.699	32.125	1.00	46.93	A
3524	CA	ASN	A1459	-20.954	-7.643	31.212	1.00	45.04	A
3525	CB	ASN	A1459	-21.200	-6.316	31.866	1.00	46.92	A
3526	CG	ASN	A1459	-20.332	-6.142	33.145	1.00	52.29	A
3527	OD1	ASN	A1459	-20.006	-7.160	33.856	1.00	46.43	A
3528	ND2	ASN	A1459	-19.887	-4.858	33.418	1.00	46.81	A
3529	C	ASN	A1459	-19.507	-7.565	31.002	1.00	42.68	A
3530	O	ASN	A1459	-19.111	-6.482	30.756	1.00	44.15	A
3531	N	LYS	A1460	-18.743	-8.638	30.964	1.00	40.59	A
3532	CA	LYS	A1460	-17.290	-8.586	30.691	1.00	42.03	A
3533	CB	LYS	A1460	-16.479	-8.473	32.092	1.00	43.56	A
3534	CG	LYS	A1460	-16.398	-7.019	32.761	1.00	39.23	A
3535	CD	LYS	A1460	-15.304	-6.988	33.808	1.00	46.14	A
3536	CE	LYS	A1460	-15.490	-7.982	34.917	1.00	49.48	A
3537	NZ	LYS	A1460	-16.531	-7.489	35.811	1.00	52.09	A
3538	C	LYS	A1460	-16.832	-9.845	29.953	1.00	39.80	A
3539	O	LYS	A1460	-17.543	-10.769	30.034	1.00	41.84	A
3540	N	VAL	A1461	-15.677	-9.953	29.309	1.00	36.19	A
3541	CA	VAL	A1461	-15.442	-11.045	28.506	1.00	34.67	A
3542	CB	VAL	A1461	-15.960	-10.765	26.946	1.00	35.29	A
3543	CG1	VAL	A1461	-14.998	-10.003	26.204	1.00	28.83	A
3544	CG2	VAL	A1461	-15.872	-11.968	26.023	1.00	36.48	A
3545	C	VAL	A1461	-13.941	-11.058	28.486	1.00	36.92	A
3546	O	VAL	A1461	-13.362	-10.079	28.612	1.00	39.29	A
3547	N	ALA	A1462	-13.280	-12.177	28.233	1.00	39.30	A
3548	CA	ALA	A1462	-11.867	-12.347	28.275	1.00	37.95	A
3549	CB	ALA	A1462	-11.634	-13.593	29.190	1.00	35.27	A
3550	C	ALA	A1462	-11.519	-12.684	26.863	1.00	38.33	A
3551	O	ALA	A1462	-12.300	-13.367	26.140	1.00	41.32	A
3552	N	ILE	A1463	-10.355	-12.396	26.405	1.00	38.51	A
3553	CA	ILE	A1463	-10.143	-12.665	24.985	1.00	38.50	A
3554	CB	ILE	A1463	-9.727	-11.348	24.332	1.00	37.98	A
3555	CG2	ILE	A1463	-9.238	-11.503	22.908	1.00	40.85	A
3556	CG1	ILE	A1463	-10.887	-10.352	24.470	1.00	36.60	A
3557	CD1	ILE	A1463	-10.579	-8.888	24.352	1.00	32.29	A
3558	C	ILE	A1463	-9.029	-13.661	24.866	1.00	39.59	A
3559	O	ILE	A1463	-7.941	-13.412	25.292	1.00	41.30	A
3560	N	LYS	A1464	-9.250	-14.790	24.254	1.00	40.49	A
3561	CA	LYS	A1464	-8.120	-15.705	23.985	1.00	40.80	A
3562	CB	LYS	A1464	-8.618	-17.126	24.294	1.00	42.62	A
3563	CG	LYS	A1464	-7.557	-17.949	25.036	1.00	39.71	A
3564	CD	LYS	A1464	-7.979	-19.502	25.172	1.00	42.55	A
3565	CE	LYS	A1464	-9.511	-19.702	25.673	1.00	45.04	A
3566	NZ	LYS	A1464	-10.052	-21.032	26.098	1.00	45.24	A
3567	C	LYS	A1464	-7.581	-15.762	22.513	1.00	41.33	A
3568	O	LYS	A1464	-8.347	-15.626	21.534	1.00	40.17	A
3569	N	VAL	A1465	-6.327	-16.191	22.369	1.00	41.36	A
3570	CA	VAL	A1465	-5.649	-16.233	21.066	1.00	40.38	A
3571	CB	VAL	A1465	-4.910	-14.849	20.840	1.00	40.98	A

3572	CG1	VAL	A1465	-4.346	-14.356	22.179	1.00	39.64	A
3573	CG2	VAL	A1465	-3.883	-14.815	19.860	1.00	35.47	A
3574	C	VAL	A1465	-4.582	-17.096	21.471	1.00	42.78	A
3575	O	VAL	A1465	-3.640	-16.664	22.051	1.00	41.85	A
3576	N	GLY	A1466	-4.696	-18.370	21.157	1.00	45.04	A
3577	CA	GLY	A1466	-3.477	-19.147	21.223	1.00	47.14	A
3578	C	GLY	A1466	-3.121	-19.781	22.526	1.00	47.56	A
3579	O	GLY	A1466	-1.873	-20.078	22.816	1.00	50.26	A
3580	N	GLY	A1467	-4.163	-20.128	23.238	1.00	46.53	A
3581	CA	GLY	A1467	-3.947	-20.807	24.452	1.00	50.31	A
3582	C	GLY	A1467	-4.282	-19.895	25.596	1.00	53.05	A
3583	O	GLY	A1467	-5.000	-20.332	26.641	1.00	53.89	A
3584	N	ARG	A1468	-3.801	-18.667	25.399	1.00	50.89	A
3585	CA	ARG	A1468	-3.748	-17.791	26.478	1.00	53.32	A
3586	CB	ARG	A1468	-2.338	-17.001	26.442	1.00	55.76	A
3587	CG	ARG	A1468	-1.073	-17.868	26.428	1.00	46.99	A
3588	CD	ARG	A1468	-1.202	-18.538	27.746	1.00	45.45	A
3589	NE	ARG	A1468	-0.471	-19.808	27.859	1.00	47.73	A
3590	CZ	ARG	A1468	0.844	-19.881	27.791	1.00	47.37	A
3591	NH1	ARG	A1468	1.563	-18.760	27.569	1.00	56.48	A
3592	NH2	ARG	A1468	1.439	-21.039	27.921	1.00	41.60	A
3593	C	ARG	A1468	-4.877	-16.807	26.359	1.00	53.13	A
3594	O	ARG	A1468	-5.372	-16.637	25.202	1.00	55.87	A
3595	N	TYR	A1469	-5.192	-16.129	27.507	1.00	51.61	A
3596	CA	TYR	A1469	-5.894	-14.814	27.587	1.00	49.46	A
3597	CB	TYR	A1469	-6.890	-14.823	28.669	1.00	50.49	A
3598	CG	TYR	A1469	-7.935	-15.937	28.756	1.00	54.68	A
3599	CD1	TYR	A1469	-9.222	-15.732	28.356	1.00	55.27	A
3600	CE1	TYR	A1469	-10.160	-16.771	28.442	1.00	58.47	A
3601	CD2	TYR	A1469	-7.623	-17.186	29.380	1.00	59.28	A
3602	CE2	TYR	A1469	-8.511	-18.226	29.452	1.00	51.69	A
3603	CZ	TYR	A1469	-9.798	-18.006	29.040	1.00	57.44	A
3604	OH	TYR	A1469	-10.747	-19.021	29.189	1.00	55.30	A
3605	C	TYR	A1469	-5.130	-13.412	27.715	1.00	48.55	A
3606	O	TYR	A1469	-4.011	-13.218	28.312	1.00	48.69	A
3607	N	LEU	A1470	-5.726	-12.445	27.056	1.00	48.34	A
3608	CA	LEU	A1470	-5.183	-11.106	26.898	1.00	49.35	A
3609	CB	LEU	A1470	-5.929	-10.282	25.900	1.00	47.63	A
3610	CG	LEU	A1470	-5.577	-10.360	24.457	1.00	44.93	A
3611	CD1	LEU	A1470	-6.481	-9.403	23.854	1.00	40.32	A
3612	CD2	LEU	A1470	-4.233	-9.826	24.289	1.00	39.91	A
3613	C	LEU	A1470	-5.396	-10.517	28.255	1.00	51.55	A
3614	O	LEU	A1470	-6.476	-10.639	28.950	1.00	51.00	A
3615	N	LYS	A1471	-4.316	-9.927	28.678	1.00	52.93	A
3616	CA	LYS	A1471	-4.345	-9.576	30.039	1.00	56.56	A
3617	CB	LYS	A1471	-4.077	-10.716	31.004	1.00	50.53	A
3618	CG	LYS	A1471	-2.685	-10.677	31.250	1.00	54.37	A
3619	CD	LYS	A1471	-2.279	-10.222	32.528	1.00	56.79	A
3620	CE	LYS	A1471	-0.764	-10.652	32.806	1.00	58.62	A
3621	NZ	LYS	A1471	-0.637	-10.969	34.322	1.00	62.92	A
3622	C	LYS	A1471	-3.300	-8.500	29.976	1.00	57.55	A
3623	O	LYS	A1471	-2.417	-8.656	29.250	1.00	59.94	A
3624	N	GLY	A1472	-3.525	-7.375	30.611	1.00	59.13	A
3625	CA	GLY	A1472	-2.647	-6.287	30.489	1.00	63.58	A
3626	C	GLY	A1472	-1.777	-6.061	31.721	1.00	66.30	A
3627	O	GLY	A1472	-2.080	-5.133	32.621	1.00	63.79	A

3628	N	ASP	A1473	-0.694	-6.890	31.685	1.00	67.87	A
3629	CA	ASP	A1473	0.444	-6.962	32.687	1.00	70.16	A
3630	CB	ASP	A1473	1.527	-7.767	32.051	1.00	70.63	A
3631	CG	ASP	A1473	1.994	-7.104	30.760	1.00	72.24	A
3632	OD1	ASP	A1473	3.260	-7.040	30.518	1.00	66.62	A
3633	OD2	ASP	A1473	1.013	-6.614	30.052	1.00	73.17	A
3634	C	ASP	A1473	1.260	-5.719	32.970	1.00	71.01	A
3635	O	ASP	A1473	0.804	-4.580	32.937	1.00	72.04	A
3636	N	HIS	A1474	2.541	-5.975	33.197	1.00	72.45	A
3637	CA	HIS	A1474	3.414	-4.899	33.559	1.00	71.88	A
3638	CB	HIS	A1474	4.766	-5.386	33.924	1.00	72.61	A
3639	CG	HIS	A1474	4.960	-5.301	35.344	1.00	71.92	A
3640	CD2	HIS	A1474	6.068	-5.181	36.106	1.00	71.89	A
3641	ND1	HIS	A1474	4.061	-5.349	36.232	1.00	72.22	A
3642	CE1	HIS	A1474	4.304	-5.274	37.431	1.00	77.40	A
3643	NE2	HIS	A1474	5.634	-5.164	37.412	1.00	78.29	A
3644	C	HIS	A1474	3.553	-3.868	32.476	1.00	72.23	A
3645	O	HIS	A1474	4.003	-4.129	31.295	1.00	69.18	A
3646	N	ALA	A1475	3.201	-2.676	32.968	1.00	70.64	A
3647	CA	ALA	A1475	3.357	-1.498	32.169	1.00	67.26	A
3648	CB	ALA	A1475	4.583	-1.680	31.170	1.00	66.74	A
3649	C	ALA	A1475	2.080	-1.146	31.468	1.00	61.44	A
3650	O	ALA	A1475	2.067	-0.145	30.792	1.00	61.89	A
3651	N	GLY	A1476	1.024	-1.873	31.734	1.00	57.05	A
3652	CA	GLY	A1476	-0.280	-1.617	31.068	1.00	53.24	A
3653	C	GLY	A1476	-0.250	-2.238	29.621	1.00	52.28	A
3654	O	GLY	A1476	-1.158	-2.055	28.870	1.00	51.59	A
3655	N	VAL	A1477	0.807	-2.939	29.207	1.00	49.69	A
3656	CA	VAL	A1477	0.851	-3.372	27.863	1.00	50.07	A
3657	CB	VAL	A1477	2.154	-4.253	27.513	1.00	50.89	A
3658	CG1	VAL	A1477	2.428	-4.245	25.949	1.00	48.16	A
3659	CG2	VAL	A1477	3.281	-3.844	28.206	1.00	45.57	A
3660	C	VAL	A1477	-0.280	-4.403	27.731	1.00	52.19	A
3661	O	VAL	A1477	-0.834	-4.872	28.801	1.00	52.43	A
3662	N	LEU	A1478	-0.539	-4.865	26.471	1.00	49.93	A
3663	CA	LEU	A1478	-1.521	-5.950	26.268	1.00	47.41	A
3664	CB	LEU	A1478	-2.612	-5.618	25.200	1.00	49.24	A
3665	CG	LEU	A1478	-3.993	-6.329	25.100	1.00	45.99	A
3666	CD1	LEU	A1478	-4.778	-6.100	26.432	1.00	51.57	A
3667	CD2	LEU	A1478	-4.949	-6.002	24.067	1.00	35.50	A
3668	C	LEU	A1478	-0.780	-7.095	25.776	1.00	48.64	A
3669	O	LEU	A1478	-0.334	-7.073	24.604	1.00	48.71	A
3670	N	LYS	A1479	-0.680	-8.137	26.605	1.00	49.41	A
3671	CA	LYS	A1479	-0.106	-9.470	26.112	1.00	50.56	A
3672	CB	LYS	A1479	1.213	-9.828	26.886	1.00	52.29	A
3673	CG	LYS	A1479	2.028	-8.684	27.466	1.00	47.09	A
3674	CD	LYS	A1479	3.250	-8.582	26.567	1.00	45.62	A
3675	CE	LYS	A1479	4.325	-7.553	26.977	1.00	46.40	A
3676	NZ	LYS	A1479	5.401	-8.350	26.313	1.00	49.55	A
3677	C	LYS	A1479	-1.069	-10.668	26.199	1.00	50.41	A
3678	O	LYS	A1479	-2.094	-10.625	26.850	1.00	52.36	A
3679	N	ALA	A1480	-0.763	-11.749	25.552	1.00	50.77	A
3680	CA	ALA	A1480	-1.536	-12.891	25.732	1.00	51.99	A
3681	CB	ALA	A1480	-1.696	-13.688	24.401	1.00	50.68	A
3682	C	ALA	A1480	-0.677	-13.678	26.680	1.00	53.93	A
3683	O	ALA	A1480	-0.246	-14.798	26.345	1.00	53.71	A

3684	N	SER	A1481	-0.568	-13.119	27.891	1.00	56.22	A
3685	CA	SER	A1481	0.114	-13.678	29.119	1.00	55.21	A
3686	CB	SER	A1481	0.855	-12.578	29.945	1.00	54.52	A
3687	OG	SER	A1481	0.237	-11.276	30.059	1.00	50.34	A
3688	C	SER	A1481	-0.782	-14.588	30.015	1.00	56.79	A
3689	O	SER	A1481	-0.419	-15.798	30.157	1.00	56.75	A
3690	N	ALA	A1482	-1.929	-14.069	30.572	1.00	54.70	A
3691	CA	ALA	A1482	-2.896	-14.912	31.398	1.00	52.31	A
3692	CB	ALA	A1482	-4.216	-14.281	31.588	1.00	46.25	A
3693	C	ALA	A1482	-3.119	-16.300	30.923	1.00	53.71	A
3694	O	ALA	A1482	-3.456	-16.574	29.692	1.00	58.22	A
3695	N	GLU	A1483	-2.950	-17.199	31.862	1.00	53.94	A
3696	CA	GLU	A1483	-3.239	-18.622	31.714	1.00	54.54	A
3697	CB	GLU	A1483	-2.079	-19.407	32.315	1.00	53.89	A
3698	CG	GLU	A1483	-2.303	-20.887	32.186	1.00	61.71	A
3699	CD	GLU	A1483	-1.338	-21.728	33.008	1.00	66.24	A
3700	OE1	GLU	A1483	-1.585	-22.967	33.133	1.00	56.00	A
3701	OE2	GLU	A1483	-0.367	-21.089	33.567	1.00	73.95	A
3702	C	GLU	A1483	-4.584	-18.899	32.427	1.00	56.07	A
3703	O	GLU	A1483	-5.386	-19.988	32.178	1.00	56.67	A
3704	N	THR	A1484	-4.935	-17.935	33.309	1.00	54.44	A
3705	CA	THR	A1484	-6.211	-18.217	33.980	1.00	53.55	A
3706	CB	THR	A1484	-6.123	-18.798	35.483	1.00	51.53	A
3707	OG1	THR	A1484	-4.793	-19.213	35.749	1.00	56.52	A
3708	CG2	THR	A1484	-6.841	-19.965	35.606	1.00	40.29	A
3709	C	THR	A1484	-6.855	-16.919	33.901	1.00	54.12	A
3710	O	THR	A1484	-6.126	-15.905	33.856	1.00	55.50	A
3711	N	VAL	A1485	-8.196	-16.925	33.951	1.00	52.19	A
3712	CA	VAL	A1485	-8.897	-15.657	33.864	1.00	51.32	A
3713	CB	VAL	A1485	-10.309	-15.715	32.985	1.00	48.19	A
3714	CG1	VAL	A1485	-10.849	-17.149	32.971	1.00	58.29	A
3715	CG2	VAL	A1485	-11.392	-14.859	33.417	1.00	40.22	A
3716	C	VAL	A1485	-8.973	-14.993	35.221	1.00	51.15	A
3717	O	VAL	A1485	-9.655	-15.479	36.110	1.00	50.77	A
3718	N	ASP	A1486	-8.368	-13.828	35.299	1.00	51.89	A
3719	CA	ASP	A1486	-8.727	-12.866	36.358	1.00	55.97	A
3720	CB	ASP	A1486	-7.485	-12.734	37.206	1.00	55.90	A
3721	CG	ASP	A1486	-6.481	-11.990	36.463	1.00	57.66	A
3722	OD1	ASP	A1486	-6.684	-10.737	36.260	1.00	62.80	A
3723	OD2	ASP	A1486	-5.616	-12.676	35.952	1.00	57.63	A
3724	C	ASP	A1486	-9.068	-11.380	35.899	1.00	56.45	A
3725	O	ASP	A1486	-8.634	-10.880	34.838	1.00	58.34	A
3726	N	PRO	A1487	-9.754	-10.656	36.741	1.00	55.84	A
3727	CD	PRO	A1487	-10.167	-11.157	38.076	1.00	57.78	A
3728	CA	PRO	A1487	-10.097	-9.276	36.648	1.00	54.70	A
3729	CB	PRO	A1487	-9.522	-8.736	38.023	1.00	54.51	A
3730	CG	PRO	A1487	-9.849	-9.910	39.007	1.00	55.62	A
3731	C	PRO	A1487	-9.427	-8.468	35.661	1.00	52.50	A
3732	O	PRO	A1487	-10.029	-7.516	35.213	1.00	51.21	A
3733	N	ALA	A1488	-8.112	-8.714	35.585	1.00	50.39	A
3734	CA	ALA	A1488	-7.133	-8.040	34.731	1.00	46.94	A
3735	CB	ALA	A1488	-5.836	-7.981	35.536	1.00	46.05	A
3736	C	ALA	A1488	-6.852	-8.805	33.309	1.00	46.32	A
3737	O	ALA	A1488	-6.090	-8.232	32.487	1.00	44.62	A
3738	N	SER	A1489	-7.323	-10.064	33.153	1.00	41.36	A
3739	CA	SER	A1489	-7.608	-10.666	31.965	1.00	45.98	A

3740	CB	SER	A1489	-7.192	-12.156	31.976	1.00	44.84	A
3741	OG	SER	A1489	-7.605	-12.779	33.160	1.00	51.52	A
3742	C	SER	A1489	-9.198	-10.596	31.503	1.00	47.24	A
3743	O	SER	A1489	-9.557	-11.193	30.398	1.00	47.31	A
3744	N	LEU	A1490	-10.062	-9.863	32.264	1.00	46.48	A
3745	CA	LEU	A1490	-11.516	-9.532	31.901	1.00	46.25	A
3746	CB	LEU	A1490	-12.472	-9.752	33.102	1.00	43.27	A
3747	CG	LEU	A1490	-12.692	-11.133	33.654	1.00	41.52	A
3748	CD1	LEU	A1490	-13.573	-11.124	34.917	1.00	31.63	A
3749	CD2	LEU	A1490	-13.415	-11.843	32.584	1.00	44.41	A
3750	C	LEU	A1490	-11.738	-8.057	31.505	1.00	46.55	A
3751	O	LEU	A1490	-11.339	-7.161	32.183	1.00	47.47	A
3752	N	TRP	A1491	-12.468	-7.828	30.457	1.00	45.90	A
3753	CA	TRP	A1491	-12.609	-6.545	29.841	1.00	45.88	A
3754	CB	TRP	A1491	-12.065	-6.635	28.385	1.00	48.02	A
3755	CG	TRP	A1491	-10.746	-7.137	28.430	1.00	45.13	A
3756	CD2	TRP	A1491	-9.658	-6.424	28.819	1.00	41.87	A
3757	CE2	TRP	A1491	-8.575	-7.284	28.773	1.00	44.90	A
3758	CE3	TRP	A1491	-9.483	-5.106	29.215	1.00	50.66	A
3759	CD1	TRP	A1491	-10.342	-8.366	28.148	1.00	49.06	A
3760	NE1	TRP	A1491	-9.029	-8.495	28.352	1.00	45.38	A
3761	CZ2	TRP	A1491	-7.321	-6.916	29.148	1.00	51.31	A
3762	CZ3	TRP	A1491	-8.200	-4.677	29.565	1.00	54.68	A
3763	CH2	TRP	A1491	-7.125	-5.590	29.525	1.00	53.89	A
3764	C	TRP	A1491	-14.117	-6.324	29.660	1.00	46.86	A
3765	O	TRP	A1491	-14.882	-7.340	29.241	1.00	43.94	A
3766	N	GLU	A1492	-14.523	-5.042	29.844	1.00	43.23	A
3767	CA	GLU	A1492	-15.873	-4.706	29.630	1.00	44.75	A
3768	CB	GLU	A1492	-16.198	-3.429	30.378	1.00	45.84	A
3769	CG	GLU	A1492	-17.488	-3.412	31.019	1.00	45.11	A
3770	CD	GLU	A1492	-17.372	-2.578	32.194	1.00	48.33	A
3771	OE1	GLU	A1492	-17.510	-1.343	32.104	1.00	55.20	A
3772	OE2	GLU	A1492	-17.074	-3.143	33.228	1.00	53.19	A
3773	C	GLU	A1492	-16.202	-4.485	28.133	1.00	42.78	A
3774	O	GLU	A1492	-15.454	-4.004	27.480	1.00	41.09	A
3775	N	TYR	A1493	-17.360	-4.780	27.598	1.00	45.74	A
3776	CA	TYR	A1493	-17.406	-4.724	26.056	1.00	46.80	A
3777	CB	TYR	A1493	-17.600	-6.073	25.549	1.00	45.31	A
3778	CG	TYR	A1493	-18.755	-6.856	26.255	1.00	45.14	A
3779	CD1	TYR	A1493	-18.463	-7.719	27.302	1.00	36.36	A
3780	CE1	TYR	A1493	-19.376	-8.522	27.879	1.00	28.95	A
3781	CD2	TYR	A1493	-20.104	-6.767	25.820	1.00	42.06	A
3782	CE2	TYR	A1493	-21.090	-7.540	26.464	1.00	38.47	A
3783	CZ	TYR	A1493	-20.692	-8.424	27.518	1.00	38.59	A
3784	OH	TYR	A1493	-21.559	-9.275	28.205	1.00	44.03	A
3785	C	TYR	A1493	-18.673	-4.014	25.716	1.00	48.11	A
3786	O	TYR	A1493	-19.306	-3.479	26.625	1.00	49.39	A
3787	OXT	TYR	A1493	-19.131	-3.914	24.653	1.00	48.37	A
3788	C	GLY	B1005	7.990	13.573	3.876	1.00	64.92	B
3789	O	GLY	B1005	9.019	14.185	4.226	1.00	64.66	B
3790	N	GLY	B1005	6.531	11.508	4.740	1.00	59.79	B
3791	CA	GLY	B1005	7.067	12.887	4.937	1.00	63.28	B
3792	N	THR	B1006	7.680	13.466	2.573	1.00	66.77	B
3793	CA	THR	B1006	8.537	14.129	1.530	1.00	67.45	B
3794	CB	THR	B1006	7.949	15.654	1.402	1.00	70.67	B
3795	OG1	THR	B1006	8.456	16.487	2.477	1.00	75.20	B

3796	CG2	THR	B1006	6.299	15.719	1.405	1.00	62.21	B
3797	C	THR	B1006	10.116	14.031	1.899	1.00	67.92	B
3798	O	THR	B1006	10.460	13.193	2.827	1.00	68.16	B
3799	N	ALA	B1007	11.080	14.764	1.273	1.00	65.04	B
3800	CA	ALA	B1007	12.410	14.921	2.053	1.00	64.21	B
3801	CB	ALA	B1007	13.685	14.922	1.129	1.00	65.26	B
3802	C	ALA	B1007	12.577	15.999	3.294	1.00	61.50	B
3803	O	ALA	B1007	13.425	16.851	3.240	1.00	57.58	B
3804	N	GLU	B1008	11.823	15.794	4.403	1.00	60.94	B
3805	CA	GLU	B1008	11.631	16.635	5.708	1.00	60.80	B
3806	CB	GLU	B1008	11.518	15.777	6.968	1.00	57.07	B
3807	CG	GLU	B1008	10.534	14.692	6.915	1.00	62.92	B
3808	CD	GLU	B1008	11.183	13.287	6.452	1.00	73.19	B
3809	OE1	GLU	B1008	12.432	13.383	6.079	1.00	73.72	B
3810	OE2	GLU	B1008	10.458	12.142	6.465	1.00	71.21	B
3811	C	GLU	B1008	12.426	17.895	6.176	1.00	58.95	B
3812	O	GLU	B1008	13.339	17.711	6.926	1.00	59.58	B
3813	N	ALA	B1009	12.037	19.131	5.774	1.00	56.80	B
3814	CA	ALA	B1009	12.356	20.364	6.521	1.00	55.01	B
3815	CB	ALA	B1009	11.715	21.515	5.835	1.00	55.05	B
3816	C	ALA	B1009	11.980	20.367	8.082	1.00	52.63	B
3817	O	ALA	B1009	11.005	19.810	8.502	1.00	50.81	B
3818	N	VAL	B1010	12.755	21.030	8.906	1.00	50.27	B
3819	CA	VAL	B1010	12.409	20.968	10.293	1.00	51.74	B
3820	CB	VAL	B1010	13.563	21.178	11.142	1.00	47.57	B
3821	CG1	VAL	B1010	14.723	20.588	10.475	1.00	45.96	B
3822	CG2	VAL	B1010	13.785	22.585	11.137	1.00	51.11	B
3823	C	VAL	B1010	11.228	21.901	10.757	1.00	53.13	B
3824	O	VAL	B1010	10.946	22.951	10.167	1.00	55.83	B
3825	N	GLN	B1011	10.578	21.454	11.820	1.00	52.10	B
3826	CA	GLN	B1011	9.512	22.091	12.463	1.00	52.38	B
3827	CB	GLN	B1011	8.441	21.115	13.075	1.00	50.75	B
3828	CG	GLN	B1011	7.108	21.939	13.424	1.00	56.95	B
3829	CD	GLN	B1011	5.739	21.204	13.695	1.00	55.34	B
3830	OE1	GLN	B1011	5.696	20.225	14.456	1.00	59.29	B
3831	NE2	GLN	B1011	4.638	21.735	13.131	1.00	46.76	B
3832	C	GLN	B1011	10.225	22.873	13.517	1.00	51.70	B
3833	O	GLN	B1011	10.380	22.365	14.583	1.00	45.52	B
3834	N	ILE	B1012	10.666	24.101	13.113	1.00	55.60	B
3835	CA	ILE	B1012	11.041	25.344	13.942	1.00	58.78	B
3836	CB	ILE	B1012	11.089	26.714	13.076	1.00	59.46	B
3837	CG2	ILE	B1012	11.495	27.857	13.913	1.00	55.23	B
3838	CG1	ILE	B1012	12.221	26.644	12.059	1.00	63.36	B
3839	CD1	ILE	B1012	13.616	25.989	12.842	1.00	57.05	B
3840	C	ILE	B1012	10.410	25.706	15.383	1.00	60.80	B
3841	O	ILE	B1012	9.276	26.234	15.459	1.00	59.41	B
3842	N	GLN	B1013	11.216	25.457	16.480	1.00	60.63	B
3843	CA	GLN	B1013	10.897	25.794	17.837	1.00	58.97	B
3844	CB	GLN	B1013	11.076	24.541	18.641	1.00	60.79	B
3845	CG	GLN	B1013	10.482	23.382	17.910	1.00	63.21	B
3846	CD	GLN	B1013	9.005	23.621	17.667	1.00	61.11	B
3847	OE1	GLN	B1013	8.135	22.783	18.041	1.00	60.59	B
3848	NE2	GLN	B1013	8.697	24.843	17.133	1.00	58.48	B
3849	C	GLN	B1013	11.795	26.783	18.473	1.00	57.78	B
3850	O	GLN	B1013	13.008	26.686	18.289	1.00	53.44	B
3851	N	PHE	B1014	11.134	27.676	19.280	1.00	58.00	B

3852	CA	PHE	B1014	11.704	28.781	20.132	1.00	56.40	B
3853	CB	PHE	B1014	12.379	29.860	19.286	1.00	58.20	B
3854	CG	PHE	B1014	11.415	30.461	18.340	1.00	62.77	B
3855	CD1	PHE	B1014	10.451	31.331	18.797	1.00	64.60	B
3856	CD2	PHE	B1014	11.371	30.020	17.001	1.00	71.90	B
3857	CE1	PHE	B1014	9.465	31.819	17.977	1.00	69.33	B
3858	CE2	PHE	B1014	10.393	30.469	16.128	1.00	73.37	B
3859	CZ	PHE	B1014	9.428	31.417	16.611	1.00	71.96	B
3860	C	PHE	B1014	10.633	29.465	21.020	1.00	55.30	B
3861	O	PHE	B1014	9.289	29.266	20.902	1.00	55.39	B
3862	N	GLY	B1015	11.191	30.313	21.905	1.00	51.23	B
3863	CA	GLY	B1015	10.374	31.096	22.818	1.00	47.34	B
3864	C	GLY	B1015	11.161	32.368	22.730	1.00	48.46	B
3865	O	GLY	B1015	12.378	32.312	22.310	1.00	47.58	B
3866	N	LEU	B1016	10.531	33.466	23.211	1.00	47.35	B
3867	CA	LEU	B1016	11.038	34.834	23.137	1.00	44.99	B
3868	CB	LEU	B1016	10.109	35.691	22.246	1.00	43.83	B
3869	CG	LEU	B1016	9.518	35.232	20.937	1.00	42.33	B
3870	CD1	LEU	B1016	10.557	34.532	19.845	1.00	37.13	B
3871	CD2	LEU	B1016	8.474	34.330	21.507	1.00	42.02	B
3872	C	LEU	B1016	10.918	35.463	24.527	1.00	46.45	B
3873	O	LEU	B1016	10.062	35.136	25.320	1.00	46.80	B
3874	N	ILE	B1017	11.676	36.469	24.794	1.00	45.92	B
3875	CA	ILE	B1017	11.656	36.867	26.094	1.00	49.57	B
3876	CB	ILE	B1017	12.961	36.248	26.964	1.00	50.38	B
3877	CG2	ILE	B1017	12.693	36.119	28.424	1.00	47.09	B
3878	CG1	ILE	B1017	13.577	35.024	26.360	1.00	49.64	B
3879	CD1	ILE	B1017	14.727	34.654	27.151	1.00	53.27	B
3880	C	ILE	B1017	11.854	38.365	26.156	1.00	50.10	B
3881	O	ILE	B1017	13.035	38.891	26.035	1.00	47.25	B
3882	N	ASN	B1018	10.757	39.022	26.489	1.00	50.92	B
3883	CA	ASN	B1018	10.871	40.466	26.669	1.00	51.32	B
3884	CB	ASN	B1018	9.491	41.109	26.965	1.00	50.40	B
3885	CG	ASN	B1018	8.943	40.690	28.291	1.00	46.54	B
3886	OD1	ASN	B1018	7.746	40.516	28.453	1.00	39.77	B
3887	ND2	ASN	B1018	9.853	40.431	29.229	1.00	48.41	B
3888	C	ASN	B1018	11.894	40.845	27.697	1.00	51.54	B
3889	O	ASN	B1018	12.676	40.074	28.062	1.00	50.58	B
3890	N	CYS	B1019	11.696	42.036	28.195	1.00	55.22	B
3891	CA	CYS	B1019	12.456	42.890	29.064	1.00	57.70	B
3892	CB	CYS	B1019	11.567	44.165	29.043	1.00	56.55	B
3893	SG	CYS	B1019	12.001	45.371	27.807	1.00	65.01	B
3894	C	CYS	B1019	12.295	42.439	30.502	1.00	58.80	B
3895	O	CYS	B1019	13.115	42.703	31.361	1.00	60.49	B
3896	N	GLY	B1020	11.122	41.955	30.837	1.00	58.81	B
3897	CA	GLY	B1020	10.831	41.653	32.208	1.00	58.81	B
3898	C	GLY	B1020	11.404	40.259	32.355	1.00	59.74	B
3899	O	GLY	B1020	11.145	39.596	33.343	1.00	60.95	B
3900	N	ASN	B1021	12.207	39.859	31.358	1.00	57.73	B
3901	CA	ASN	B1021	12.808	38.571	31.242	1.00	56.47	B
3902	CB	ASN	B1021	13.832	38.263	32.256	1.00	54.86	B
3903	CG	ASN	B1021	15.193	38.718	31.805	1.00	59.85	B
3904	OD1	ASN	B1021	16.038	39.103	32.602	1.00	60.36	B
3905	ND2	ASN	B1021	15.423	38.713	30.487	1.00	66.68	B
3906	C	ASN	B1021	11.881	37.526	31.252	1.00	57.35	B
3907	O	ASN	B1021	12.305	36.464	31.428	1.00	62.51	B

3908	N	LYS	B1022	10.625	37.759	31.013	1.00	57.77	B
3909	CA	LYS	B1022	9.603	36.766	31.149	1.00	57.49	B
3910	CB	LYS	B1022	8.459	37.546	31.651	1.00	59.48	B
3911	CG	LYS	B1022	7.950	37.060	32.943	1.00	60.86	B
3912	CD	LYS	B1022	8.944	37.431	34.053	1.00	59.38	B
3913	CE	LYS	B1022	8.736	38.851	34.631	1.00	47.42	B
3914	NZ	LYS	B1022	7.271	38.818	35.030	1.00	42.36	B
3915	C	LYS	B1022	9.249	36.287	29.749	1.00	58.01	B
3916	O	LYS	B1022	9.870	36.825	28.806	1.00	58.90	B
3917	N	TYR	B1023	8.272	35.361	29.603	1.00	56.71	B
3918	CA	TYR	B1023	8.055	34.478	28.372	1.00	55.35	B
3919	CB	TYR	B1023	8.273	32.988	28.655	1.00	55.47	B
3920	CG	TYR	B1023	9.700	32.544	28.519	1.00	54.08	B
3921	CD1	TYR	B1023	10.519	32.491	29.614	1.00	54.83	B
3922	CE1	TYR	B1023	11.869	32.175	29.513	1.00	53.53	B
3923	CD2	TYR	B1023	10.203	32.177	27.322	1.00	48.63	B
3924	CE2	TYR	B1023	11.535	31.900	27.180	1.00	52.63	B
3925	CZ	TYR	B1023	12.395	31.916	28.303	1.00	52.61	B
3926	OH	TYR	B1023	13.766	31.593	28.229	1.00	51.96	B
3927	C	TYR	B1023	6.697	34.426	27.722	1.00	55.90	B
3928	O	TYR	B1023	5.653	34.016	28.338	1.00	54.90	B
3929	N	LEU	B1024	6.715	34.733	26.436	1.00	56.47	B
3930	CA	LEU	B1024	5.528	34.589	25.635	1.00	57.39	B
3931	CB	LEU	B1024	5.984	34.633	24.273	1.00	54.25	B
3932	CG	LEU	B1024	5.283	35.735	23.588	1.00	57.27	B
3933	CD1	LEU	B1024	3.482	35.743	23.281	1.00	46.48	B
3934	CD2	LEU	B1024	5.856	36.854	24.488	1.00	53.35	B
3935	C	LEU	B1024	4.781	33.257	25.824	1.00	60.67	B
3936	O	LEU	B1024	5.323	32.152	25.452	1.00	61.55	B
3937	N	THR	B1025	3.552	33.317	26.384	1.00	63.02	B
3938	CA	THR	B1025	2.949	32.094	26.942	1.00	65.23	B
3939	CB	THR	B1025	3.242	31.904	28.567	1.00	65.80	B
3940	OG1	THR	B1025	4.625	31.585	28.883	1.00	65.20	B
3941	CG2	THR	B1025	2.450	30.784	29.169	1.00	64.50	B
3942	C	THR	B1025	1.465	31.958	26.648	1.00	66.64	B
3943	O	THR	B1025	0.712	32.817	26.965	1.00	68.11	B
3944	N	ALA	B1026	1.043	30.834	26.095	1.00	69.67	B
3945	CA	ALA	B1026	-0.357	30.628	25.627	1.00	72.14	B
3946	CB	ALA	B1026	-0.432	29.672	24.299	1.00	71.38	B
3947	C	ALA	B1026	-1.338	30.163	26.723	1.00	72.69	B
3948	O	ALA	B1026	-2.359	29.440	26.434	1.00	73.33	B
3949	N	GLU	B1027	-1.082	30.697	27.928	1.00	73.46	B
3950	CA	GLU	B1027	-1.721	30.257	29.210	1.00	73.22	B
3951	CB	GLU	B1027	-1.486	31.208	30.452	1.00	73.20	B
3952	CG	GLU	B1027	-0.080	31.191	31.229	1.00	70.78	B
3953	CD	GLU	B1027	0.235	29.964	32.077	1.00	69.66	B
3954	OE1	GLU	B1027	1.414	29.905	32.611	1.00	62.43	B
3955	OE2	GLU	B1027	-0.688	29.062	32.194	1.00	67.75	B
3956	C	GLU	B1027	-3.204	29.870	29.157	1.00	73.10	B
3957	O	GLU	B1027	-4.063	30.521	28.496	1.00	71.46	B
3958	N	ALA	B1028	-3.374	28.707	29.804	1.00	73.85	B
3959	CA	ALA	B1028	-4.545	28.156	30.514	1.00	74.31	B
3960	CB	ALA	B1028	-4.145	27.891	32.072	1.00	73.59	B
3961	C	ALA	B1028	-5.918	28.868	30.417	1.00	73.94	B
3962	O	ALA	B1028	-6.958	28.274	30.209	1.00	69.99	B
3963	N	PHE	B1029	-5.851	30.159	30.732	1.00	77.81	B

3964	CA	PHE	B1029	-6.961	31.165	30.641	1.00	77.44	B
3965	CB	PHE	B1029	-6.667	32.367	31.633	1.00	78.64	B
3966	CG	PHE	B1029	-6.854	31.987	33.189	1.00	79.84	B
3967	CD1	PHE	B1029	-5.746	31.533	33.984	1.00	80.64	B
3968	CD2	PHE	B1029	-8.130	32.115	33.842	1.00	82.05	B
3969	CE1	PHE	B1029	-5.876	31.163	35.382	1.00	80.19	B
3970	CE2	PHE	B1029	-8.299	31.734	35.274	1.00	81.97	B
3971	CZ	PHE	B1029	-7.155	31.248	36.032	1.00	80.47	B
3972	C	PHE	B1029	-7.205	31.397	29.098	1.00	75.84	B
3973	O	PHE	B1029	-6.275	31.839	28.322	1.00	74.53	B
3974	N	GLY	B1030	-8.402	30.929	28.674	1.00	75.62	B
3975	CA	GLY	B1030	-8.652	30.462	27.280	1.00	75.55	B
3976	C	GLY	B1030	-8.545	31.816	26.544	1.00	77.49	B
3977	O	GLY	B1030	-9.149	32.834	27.055	1.00	79.63	B
3978	N	PHE	B1031	-7.786	31.897	25.428	1.00	74.40	B
3979	CA	PHE	B1031	-7.589	33.208	24.690	1.00	72.75	B
3980	CB	PHE	B1031	-8.846	34.046	24.387	1.00	68.24	B
3981	CG	PHE	B1031	-9.837	33.363	23.486	1.00	69.64	B
3982	CD1	PHE	B1031	-11.132	33.960	23.281	1.00	67.89	B
3983	CD2	PHE	B1031	-9.533	32.105	22.874	1.00	61.32	B
3984	CE1	PHE	B1031	-12.104	33.316	22.457	1.00	63.21	B
3985	CE2	PHE	B1031	-10.495	31.430	22.138	1.00	64.99	B
3986	CZ	PHE	B1031	-11.786	32.004	21.914	1.00	65.65	B
3987	C	PHE	B1031	-6.493	34.082	25.324	1.00	72.75	B
3988	O	PHE	B1031	-6.683	35.264	25.541	1.00	73.78	B
3989	N	LYS	B1032	-5.327	33.536	25.587	1.00	71.01	B
3990	CA	LYS	B1032	-4.342	34.402	26.136	1.00	70.20	B
3991	CB	LYS	B1032	-3.939	34.083	27.620	1.00	70.09	B
3992	CG	LYS	B1032	-5.143	34.146	28.684	1.00	72.33	B
3993	CD	LYS	B1032	-6.079	35.438	28.598	1.00	74.05	B
3994	CE	LYS	B1032	-7.440	35.510	29.516	1.00	68.63	B
3995	NZ	LYS	B1032	-7.203	35.651	30.978	1.00	60.84	B
3996	C	LYS	B1032	-3.301	34.050	25.215	1.00	69.02	B
3997	O	LYS	B1032	-3.282	32.899	24.723	1.00	70.12	B
3998	N	VAL	B1033	-2.466	35.058	24.971	1.00	66.85	B
3999	CA	VAL	B1033	-1.223	35.044	24.239	1.00	64.30	B
4000	CB	VAL	B1033	-1.343	36.107	22.996	1.00	64.56	B
4001	CG1	VAL	B1033	-1.310	37.515	23.495	1.00	70.02	B
4002	CG2	VAL	B1033	-0.283	36.024	21.912	1.00	59.73	B
4003	C	VAL	B1033	-0.284	35.545	25.295	1.00	62.81	B
4004	O	VAL	B1033	0.862	35.687	25.009	1.00	62.29	B
4005	N	ASN	B1034	-0.797	35.815	26.517	1.00	61.89	B
4006	CA	ASN	B1034	-0.101	36.655	27.521	1.00	61.82	B
4007	CB	ASN	B1034	-0.537	36.492	28.959	1.00	60.74	B
4008	CG	ASN	B1034	0.095	35.227	29.590	1.00	64.06	B
4009	OD1	ASN	B1034	1.324	35.197	30.012	1.00	55.00	B
4010	ND2	ASN	B1034	-0.754	34.113	29.600	1.00	65.02	B
4011	C	ASN	B1034	1.341	36.354	27.554	1.00	62.16	B
4012	O	ASN	B1034	1.695	35.224	27.080	1.00	61.69	B
4013	N	ALA	B1035	2.149	37.299	28.134	1.00	60.81	B
4014	CA	ALA	B1035	3.551	36.953	28.387	1.00	61.41	B
4015	CB	ALA	B1035	4.482	37.894	27.713	1.00	62.19	B
4016	C	ALA	B1035	3.878	36.785	29.881	1.00	61.65	B
4017	O	ALA	B1035	4.521	37.739	30.543	1.00	61.26	B
4018	N	SER	B1036	3.398	35.645	30.423	1.00	59.46	B
4019	CA	SER	B1036	3.604	35.291	31.913	1.00	61.03	B

4020	CB	SER	B1036	2.340	35.158	32.752	1.00	59.54	B
4021	OG	SER	B1036	1.616	36.464	32.653	1.00	62.07	B
4022	C	SER	B1036	4.748	34.345	32.298	1.00	60.45	B
4023	O	SER	B1036	5.877	34.947	32.488	1.00	62.38	B
4024	N	ALA	B1037	4.578	32.987	32.364	1.00	56.13	B
4025	CA	ALA	B1037	5.783	32.200	32.638	1.00	56.29	B
4026	CB	ALA	B1037	5.711	30.953	31.927	1.00	58.17	B
4027	C	ALA	B1037	7.308	32.825	32.503	1.00	56.52	B
4028	O	ALA	B1037	7.593	33.692	31.654	1.00	56.41	B
4029	N	SER	B1038	8.289	32.333	33.296	1.00	54.68	B
4030	CA	SER	B1038	9.589	32.970	33.360	1.00	52.82	B
4031	CB	SER	B1038	9.838	33.411	34.746	1.00	51.93	B
4032	OG	SER	B1038	9.150	32.542	35.680	1.00	57.79	B
4033	C	SER	B1038	10.592	31.949	33.174	1.00	52.83	B
4034	O	SER	B1038	11.884	32.212	33.370	1.00	54.23	B
4035	N	SER	B1039	10.113	30.744	32.868	1.00	51.78	B
4036	CA	SER	B1039	11.044	29.648	32.548	1.00	51.19	B
4037	CB	SER	B1039	10.786	28.585	33.571	1.00	50.89	B
4038	OG	SER	B1039	11.882	28.230	34.306	1.00	52.43	B
4039	C	SER	B1039	10.540	29.184	31.188	1.00	52.10	B
4040	O	SER	B1039	9.290	29.089	31.002	1.00	53.61	B
4041	N	LEU	B1040	11.391	28.834	30.225	1.00	52.66	B
4042	CA	LEU	B1040	10.776	28.398	28.944	1.00	53.05	B
4043	CB	LEU	B1040	11.740	28.702	27.744	1.00	53.94	B
4044	CG	LEU	B1040	11.555	28.372	26.190	1.00	52.12	B
4045	CD1	LEU	B1040	12.802	28.739	25.590	1.00	48.44	B
4046	CD2	LEU	B1040	11.178	26.891	25.780	1.00	39.54	B
4047	C	LEU	B1040	10.393	26.944	28.899	1.00	53.66	B
4048	O	LEU	B1040	11.252	26.124	28.710	1.00	55.90	B
4049	N	LYS	B1041	9.116	26.596	28.974	1.00	55.00	B
4050	CA	LYS	B1041	8.677	25.195	28.800	1.00	54.92	B
4051	CB	LYS	B1041	8.561	24.460	30.115	1.00	55.47	B
4052	CG	LYS	B1041	9.557	24.808	31.296	1.00	57.58	B
4053	CD	LYS	B1041	9.203	23.905	32.455	1.00	52.69	B
4054	CE	LYS	B1041	9.808	22.419	32.321	1.00	54.24	B
4055	NZ	LYS	B1041	10.878	22.068	31.294	1.00	42.28	B
4056	C	LYS	B1041	7.258	25.203	28.214	1.00	58.11	B
4057	O	LYS	B1041	6.486	26.082	28.520	1.00	59.47	B
4058	N	LYS	B1042	6.870	24.164	27.456	1.00	60.17	B
4059	CA	LYS	B1042	5.465	23.987	27.034	1.00	59.01	B
4060	CB	LYS	B1042	4.492	23.616	28.194	1.00	57.96	B
4061	CG	LYS	B1042	4.342	22.099	28.660	1.00	57.77	B
4062	CD	LYS	B1042	5.572	21.690	29.741	1.00	62.73	B
4063	CE	LYS	B1042	5.212	22.167	31.255	1.00	58.09	B
4064	NZ	LYS	B1042	5.238	23.627	31.551	1.00	58.72	B
4065	C	LYS	B1042	4.962	25.270	26.442	1.00	59.29	B
4066	O	LYS	B1042	5.409	25.779	25.370	1.00	60.85	B
4067	N	LYS	B1043	4.027	25.794	27.197	1.00	58.90	B
4068	CA	LYS	B1043	3.087	26.850	26.778	1.00	59.81	B
4069	CB	LYS	B1043	2.334	27.287	28.007	1.00	58.15	B
4070	CG	LYS	B1043	1.393	26.229	28.579	1.00	60.55	B
4071	CD	LYS	B1043	1.025	26.629	30.093	1.00	61.33	B
4072	CE	LYS	B1043	2.085	26.020	31.119	1.00	61.66	B
4073	NZ	LYS	B1043	3.410	25.831	30.300	1.00	48.96	B
4074	C	LYS	B1043	3.729	28.064	26.010	1.00	59.15	B
4075	O	LYS	B1043	3.035	28.789	25.352	1.00	59.64	B

4076	N	GLN	B1044	5.063	28.169	26.135	1.00	60.75	B
4077	CA	GLN	B1044	6.072	29.046	25.505	1.00	60.34	B
4078	CB	GLN	B1044	7.128	29.288	26.510	1.00	58.68	B
4079	CG	GLN	B1044	6.484	30.202	27.578	1.00	64.28	B
4080	CD	GLN	B1044	6.273	29.537	28.894	1.00	57.55	B
4081	OE1	GLN	B1044	7.278	29.127	29.546	1.00	56.30	B
4082	NE2	GLN	B1044	4.980	29.329	29.234	1.00	40.71	B
4083	C	GLN	B1044	6.878	28.433	24.431	1.00	60.51	B
4084	O	GLN	B1044	7.950	28.967	24.095	1.00	59.01	B
4085	N	ILE	B1045	6.459	27.293	23.883	1.00	61.21	B
4086	CA	ILE	B1045	7.241	26.956	22.693	1.00	60.75	B
4087	CB	ILE	B1045	7.607	25.468	22.523	1.00	59.58	B
4088	CG2	ILE	B1045	9.092	25.117	23.008	1.00	54.32	B
4089	CG1	ILE	B1045	6.477	24.595	22.973	1.00	54.86	B
4090	CD1	ILE	B1045	6.829	23.236	22.640	1.00	56.07	B
4091	C	ILE	B1045	6.384	27.425	21.513	1.00	63.20	B
4092	O	ILE	B1045	5.125	27.133	21.460	1.00	64.50	B
4093	N	TRP	B1046	7.012	28.178	20.623	1.00	61.68	B
4094	CA	TRP	B1046	6.201	28.684	19.570	1.00	63.72	B
4095	CB	TRP	B1046	6.209	30.280	19.624	1.00	66.18	B
4096	CG	TRP	B1046	5.329	30.895	20.685	1.00	65.67	B
4097	CD2	TRP	B1046	3.969	31.334	20.529	1.00	70.73	B
4098	CE2	TRP	B1046	3.551	31.828	21.812	1.00	68.49	B
4099	CE3	TRP	B1046	3.039	31.336	19.439	1.00	69.96	B
4100	CD1	TRP	B1046	5.684	31.174	21.974	1.00	65.18	B
4101	NE1	TRP	B1046	4.628	31.695	22.656	1.00	66.91	B
4102	CZ2	TRP	B1046	2.216	32.300	22.080	1.00	65.15	B
4103	CZ3	TRP	B1046	1.698	31.855	19.692	1.00	68.43	B
4104	CH2	TRP	B1046	1.308	32.304	21.049	1.00	66.39	B
4105	C	TRP	B1046	6.879	28.151	18.315	1.00	63.04	B
4106	O	TRP	B1046	8.150	28.214	18.293	1.00	63.78	B
4107	N	THR	B1047	6.124	27.643	17.313	1.00	61.17	B
4108	CA	THR	B1047	6.759	27.358	15.973	1.00	62.06	B
4109	CB	THR	B1047	6.550	25.960	15.513	1.00	63.12	B
4110	OG1	THR	B1047	6.693	25.112	16.677	1.00	64.91	B
4111	CG2	THR	B1047	7.542	25.485	14.189	1.00	59.96	B
4112	C	THR	B1047	6.517	28.288	14.784	1.00	64.10	B
4113	O	THR	B1047	5.526	28.135	14.057	1.00	67.36	B
4114	N	ALA	B1058	7.306	36.366	1.705	1.00	65.68	B
4115	CA	ALA	B1058	8.233	37.129	2.494	1.00	65.53	B
4116	CB	ALA	B1058	8.618	38.441	1.775	1.00	65.75	B
4117	C	ALA	B1058	7.692	37.434	3.917	1.00	64.37	B
4118	O	ALA	B1058	7.292	38.552	4.144	1.00	65.87	B
4119	N	ALA	B1059	7.743	36.490	4.856	1.00	61.82	B
4120	CA	ALA	B1059	6.895	36.535	6.030	1.00	61.03	B
4121	CB	ALA	B1059	5.581	36.911	5.579	1.00	61.18	B
4122	C	ALA	B1059	6.706	35.210	6.769	1.00	62.05	B
4123	O	ALA	B1059	6.782	34.173	6.131	1.00	61.35	B
4124	N	VAL	B1060	6.280	35.245	8.063	1.00	63.12	B
4125	CA	VAL	B1060	5.865	34.039	8.832	1.00	60.28	B
4126	CB	VAL	B1060	7.072	33.526	9.634	1.00	61.30	B
4127	CG1	VAL	B1060	8.009	32.879	8.807	1.00	54.83	B
4128	CG2	VAL	B1060	7.719	34.581	10.358	1.00	60.86	B
4129	C	VAL	B1060	4.611	33.919	9.784	1.00	61.02	B
4130	O	VAL	B1060	4.335	34.702	10.713	1.00	62.87	B
4131	N	CYS	B1061	3.924	32.810	9.682	1.00	61.05	B

4132	CA	CYS	B1061	3.029	32.382	10.766	1.00	62.44	B
4133	CB	CYS	B1061	2.058	31.371	10.182	1.00	63.38	B
4134	SG	CYS	B1061	1.385	32.179	8.752	1.00	68.62	B
4135	C	CYS	B1061	3.717	31.829	12.071	1.00	61.99	B
4136	O	CYS	B1061	4.964	31.716	12.187	1.00	61.55	B
4137	N	LEU	B1062	2.914	31.508	13.065	1.00	60.64	B
4138	CA	LEU	B1062	3.432	31.343	14.459	1.00	59.10	B
4139	CB	LEU	B1062	4.090	32.623	14.970	1.00	57.14	B
4140	CG	LEU	B1062	5.621	32.632	15.273	1.00	49.68	B
4141	CD1	LEU	B1062	6.601	32.439	14.341	1.00	51.30	B
4142	CD2	LEU	B1062	5.957	33.976	15.609	1.00	48.78	B
4143	C	LEU	B1062	2.250	30.818	15.341	1.00	59.81	B
4144	O	LEU	B1062	1.233	31.455	15.573	1.00	57.04	B
4145	N	ARG	B1063	2.369	29.546	15.700	1.00	61.95	B
4146	CA	ARG	B1063	1.216	28.799	16.246	1.00	62.88	B
4147	CB	ARG	B1063	0.933	27.526	15.343	1.00	64.18	B
4148	CG	ARG	B1063	-0.535	26.961	15.374	1.00	63.24	B
4149	CD	ARG	B1063	-0.686	25.426	14.867	1.00	64.29	B
4150	NE	ARG	B1063	0.415	24.501	15.185	1.00	59.18	B
4151	CZ	ARG	B1063	0.203	23.410	15.952	1.00	68.64	B
4152	NH1	ARG	B1063	-1.065	23.205	16.375	1.00	66.47	B
4153	NH2	ARG	B1063	1.210	22.511	16.300	1.00	67.00	B
4154	C	ARG	B1063	1.434	28.482	17.742	1.00	61.65	B
4155	O	ARG	B1063	2.539	28.092	18.151	1.00	57.28	B
4156	N	SER	B1064	0.385	28.761	18.540	1.00	63.75	B
4157	CA	SER	B1064	0.332	28.223	19.928	1.00	67.35	B
4158	CB	SER	B1064	-0.939	28.671	20.736	1.00	68.21	B
4159	OG	SER	B1064	-2.206	28.827	19.985	1.00	74.70	B
4160	C	SER	B1064	0.658	26.647	20.067	1.00	67.70	B
4161	O	SER	B1064	1.123	25.909	19.119	1.00	65.91	B
4162	N	HIS	B1065	0.499	26.202	21.297	1.00	67.03	B
4163	CA	HIS	B1065	0.730	24.854	21.620	1.00	67.26	B
4164	CB	HIS	B1065	1.100	24.685	23.099	1.00	66.20	B
4165	CG	HIS	B1065	1.039	23.264	23.543	1.00	68.34	B
4166	CD2	HIS	B1065	0.032	22.557	24.128	1.00	63.90	B
4167	ND1	HIS	B1065	2.073	22.360	23.326	1.00	66.82	B
4168	CE1	HIS	B1065	1.719	21.174	23.805	1.00	62.66	B
4169	NE2	HIS	B1065	0.471	21.252	24.253	1.00	57.22	B
4170	C	HIS	B1065	-0.639	24.286	21.330	1.00	69.08	B
4171	O	HIS	B1065	-0.827	23.048	21.298	1.00	70.98	B
4172	N	LEU	B1066	-1.613	25.171	21.071	1.00	68.60	B
4173	CA	LEU	B1066	-2.961	24.712	21.175	1.00	67.86	B
4174	CB	LEU	B1066	-3.676	25.713	22.045	1.00	67.54	B
4175	CG	LEU	B1066	-3.111	25.389	23.481	1.00	66.72	B
4176	CD1	LEU	B1066	-3.707	26.230	24.637	1.00	56.75	B
4177	CD2	LEU	B1066	-3.226	23.815	23.792	1.00	64.51	B
4178	C	LEU	B1066	-3.737	24.261	19.875	1.00	68.67	B
4179	O	LEU	B1066	-4.862	23.650	19.944	1.00	69.10	B
4180	N	GLY	B1067	-3.139	24.478	18.705	1.00	66.95	B
4181	CA	GLY	B1067	-4.020	24.713	17.596	1.00	65.56	B
4182	C	GLY	B1067	-3.688	25.976	16.744	1.00	65.90	B
4183	O	GLY	B1067	-3.534	25.845	15.481	1.00	64.00	B
4184	N	ARG	B1068	-3.523	27.140	17.434	1.00	66.07	B
4185	CA	ARG	B1068	-3.941	28.538	16.965	1.00	65.03	B
4186	CB	ARG	B1068	-4.671	29.327	18.123	1.00	68.37	B
4187	CG	ARG	B1068	-5.489	28.507	19.395	1.00	72.19	B

4188	CD	ARG	B1068	-6.736	29.219	20.333	1.00	66.71	B
4189	NE	ARG	B1068	-6.684	28.718	21.730	1.00	72.55	B
4190	CZ	ARG	B1068	-6.970	29.389	22.888	1.00	77.20	B
4191	NH1	ARG	B1068	-7.437	30.676	22.890	1.00	77.35	B
4192	NH2	ARG	B1068	-6.813	28.763	24.098	1.00	70.39	B
4193	C	ARG	B1068	-2.779	29.404	16.448	1.00	62.90	B
4194	O	ARG	B1068	-1.614	29.164	16.793	1.00	63.68	B
4195	N	TYR	B1069	-3.033	30.419	15.649	1.00	60.34	B
4196	CA	TYR	B1069	-1.881	31.417	15.247	1.00	59.14	B
4197	CB	TYR	B1069	-1.706	31.414	13.655	1.00	57.35	B
4198	CG	TYR	B1069	-1.616	29.895	13.124	1.00	57.33	B
4199	CD1	TYR	B1069	-0.512	29.348	12.469	1.00	56.02	B
4200	CE1	TYR	B1069	-0.497	27.960	12.040	1.00	54.72	B
4201	CD2	TYR	B1069	-2.621	28.998	13.370	1.00	60.37	B
4202	CE2	TYR	B1069	-2.539	27.658	12.959	1.00	57.17	B
4203	CZ	TYR	B1069	-1.510	27.136	12.327	1.00	53.31	B
4204	OH	TYR	B1069	-1.612	25.712	12.006	1.00	52.16	B
4205	C	TYR	B1069	-1.877	32.880	16.034	1.00	58.97	B
4206	O	TYR	B1069	-2.986	33.361	16.552	1.00	60.02	B
4207	N	LEU	B1070	-0.697	33.502	16.226	1.00	55.25	B
4208	CA	LEU	B1070	-0.585	34.885	16.670	1.00	52.60	B
4209	CB	LEU	B1070	0.863	35.339	16.697	1.00	49.85	B
4210	CG	LEU	B1070	1.085	36.357	17.817	1.00	48.54	B
4211	CD1	LEU	B1070	0.501	35.667	19.294	1.00	48.88	B
4212	CD2	LEU	B1070	2.458	36.843	18.016	1.00	41.09	B
4213	C	LEU	B1070	-1.219	35.705	15.611	1.00	52.06	B
4214	O	LEU	B1070	-1.151	35.265	14.496	1.00	52.13	B
4215	N	ALA	B1071	-1.759	36.898	15.947	1.00	52.27	B
4216	CA	ALA	B1071	-2.523	37.801	15.038	1.00	51.52	B
4217	CB	ALA	B1071	-3.854	37.291	14.857	1.00	50.61	B
4218	C	ALA	B1071	-2.681	39.213	15.539	1.00	51.87	B
4219	O	ALA	B1071	-3.630	39.507	16.261	1.00	51.87	B
4220	N	ALA	B1072	-1.777	40.086	15.138	1.00	52.44	B
4221	CA	ALA	B1072	-1.904	41.565	15.468	1.00	53.12	B
4222	CB	ALA	B1072	-0.455	42.196	15.565	1.00	50.42	B
4223	C	ALA	B1072	-2.777	42.418	14.441	1.00	52.44	B
4224	O	ALA	B1072	-2.390	42.674	13.319	1.00	56.95	B
4225	N	ASP	B1073	-3.918	42.871	14.805	1.00	49.72	B
4226	CA	ASP	B1073	-4.743	43.591	13.937	1.00	48.78	B
4227	CB	ASP	B1073	-6.137	43.521	14.517	1.00	47.79	B
4228	CG	ASP	B1073	-6.331	44.374	15.670	1.00	43.29	B
4229	OD1	ASP	B1073	-5.534	45.213	16.012	1.00	45.27	B
4230	OD2	ASP	B1073	-7.334	44.241	16.269	1.00	49.39	B
4231	C	ASP	B1073	-4.416	45.052	13.851	1.00	51.18	B
4232	O	ASP	B1073	-3.441	45.537	14.481	1.00	51.00	B
4233	N	LYS	B1074	-5.325	45.763	13.137	1.00	50.80	B
4234	CA	LYS	B1074	-5.168	47.177	12.895	1.00	52.35	B
4235	CB	LYS	B1074	-6.381	47.788	12.172	1.00	51.89	B
4236	CG	LYS	B1074	-6.100	49.287	11.948	1.00	48.25	B
4237	CD	LYS	B1074	-5.875	49.636	10.434	1.00	55.99	B
4238	CE	LYS	B1074	-4.360	49.606	9.907	1.00	55.77	B
4239	NZ	LYS	B1074	-4.350	49.522	8.425	1.00	52.33	B
4240	C	LYS	B1074	-4.880	48.101	14.085	1.00	53.30	B
4241	O	LYS	B1074	-4.348	49.131	13.841	1.00	57.61	B
4242	N	ASP	B1075	-5.317	47.825	15.284	1.00	53.09	B
4243	CA	ASP	B1075	-5.251	48.753	16.339	1.00	55.33	B

4244	CB	ASP	B1075	-6.635	49.012	16.957	1.00	54.01	B
4245	CG	ASP	B1075	-7.786	49.218	15.901	1.00	54.40	B
4246	OD1	ASP	B1075	-8.724	48.411	16.022	1.00	50.97	B
4247	OD2	ASP	B1075	-7.798	50.171	15.005	1.00	47.78	B
4248	C	ASP	B1075	-4.346	48.146	17.435	1.00	58.52	B
4249	O	ASP	B1075	-4.369	48.624	18.656	1.00	60.90	B
4250	N	GLY	B1076	-3.607	47.066	17.053	1.00	59.04	B
4251	CA	GLY	B1076	-2.483	46.443	17.865	1.00	56.50	B
4252	C	GLY	B1076	-2.923	45.319	18.795	1.00	55.19	B
4253	O	GLY	B1076	-2.236	44.942	19.732	1.00	53.05	B
4254	N	ASN	B1077	-4.081	44.805	18.470	1.00	54.96	B
4255	CA	ASN	B1077	-4.721	43.869	19.225	1.00	57.48	B
4256	CB	ASN	B1077	-6.136	43.946	18.882	1.00	54.71	B
4257	CG	ASN	B1077	-6.914	44.969	19.758	1.00	61.91	B
4258	OD1	ASN	B1077	-8.208	44.898	19.812	1.00	60.83	B
4259	ND2	ASN	B1077	-6.173	45.950	20.437	1.00	57.19	B
4260	C	ASN	B1077	-4.133	42.413	19.061	1.00	61.30	B
4261	O	ASN	B1077	-4.485	41.668	18.083	1.00	61.06	B
4262	N	VAL	B1078	-3.303	41.978	20.080	1.00	62.27	B
4263	CA	VAL	B1078	-2.350	40.940	19.803	1.00	62.80	B
4264	CB	VAL	B1078	-1.069	41.283	20.344	1.00	62.28	B
4265	CG1	VAL	B1078	-0.011	40.276	19.991	1.00	62.88	B
4266	CG2	VAL	B1078	-0.624	42.518	19.672	1.00	64.07	B
4267	C	VAL	B1078	-2.851	39.635	20.270	1.00	65.30	B
4268	O	VAL	B1078	-3.066	39.442	21.510	1.00	65.74	B
4269	N	THR	B1079	-3.029	38.717	19.282	1.00	66.85	B
4270	CA	THR	B1079	-3.784	37.415	19.581	1.00	69.02	B
4271	CB	THR	B1079	-5.225	37.333	19.058	1.00	68.35	B
4272	OG1	THR	B1079	-5.587	38.601	18.552	1.00	76.10	B
4273	CG2	THR	B1079	-6.132	37.002	20.142	1.00	72.01	B
4274	C	THR	B1079	-3.157	36.146	19.053	1.00	67.90	B
4275	O	THR	B1079	-2.138	36.206	18.358	1.00	66.97	B
4276	N	CYS	B1080	-3.848	35.041	19.401	1.00	68.61	B
4277	CA	CYS	B1080	-3.474	33.639	19.181	1.00	69.78	B
4278	CB	CYS	B1080	-2.620	33.132	20.378	1.00	69.20	B
4279	SG	CYS	B1080	-1.616	31.805	19.673	1.00	70.02	B
4280	C	CYS	B1080	-4.763	32.839	19.026	1.00	70.72	B
4281	O	CYS	B1080	-5.008	31.879	19.751	1.00	71.53	B
4282	N	GLU	B1081	-5.677	33.298	18.157	1.00	72.40	B
4283	CA	GLU	B1081	-7.017	32.678	18.125	1.00	72.00	B
4284	CB	GLU	B1081	-8.015	33.446	18.998	1.00	73.32	B
4285	CG	GLU	B1081	-7.702	34.940	19.350	1.00	72.12	B
4286	CD	GLU	B1081	-8.810	35.626	20.295	1.00	72.68	B
4287	OE1	GLU	B1081	-8.574	36.787	20.706	1.00	71.94	B
4288	OE2	GLU	B1081	-9.921	35.060	20.624	1.00	76.69	B
4289	C	GLU	B1081	-7.597	32.316	16.746	1.00	71.26	B
4290	O	GLU	B1081	-8.843	32.115	16.591	1.00	68.77	B
4291	N	ARG	B1082	-6.672	32.242	15.773	1.00	71.36	B
4292	CA	ARG	B1082	-6.977	31.955	14.309	1.00	71.52	B
4293	CB	ARG	B1082	-6.777	33.121	13.294	1.00	69.86	B
4294	CG	ARG	B1082	-5.556	34.019	13.582	1.00	73.94	B
4295	CD	ARG	B1082	-5.628	35.454	12.954	1.00	70.48	B
4296	NE	ARG	B1082	-6.857	36.193	13.343	1.00	68.79	B
4297	CZ	ARG	B1082	-7.401	37.153	12.588	1.00	59.85	B
4298	NH1	ARG	B1082	-6.779	37.411	11.481	1.00	56.41	B
4299	NH2	ARG	B1082	-8.516	37.830	12.974	1.00	53.47	B

4300	C	ARG	B1082	-6.217	30.754	13.883	1.00	71.79	B
4301	O	ARG	B1082	-5.151	30.833	13.176	1.00	73.06	B
4302	N	GLU	B1083	-6.789	29.654	14.379	1.00	71.70	B
4303	CA	GLU	B1083	-6.569	28.224	13.920	1.00	71.18	B
4304	CB	GLU	B1083	-7.813	27.372	14.255	1.00	69.91	B
4305	CG	GLU	B1083	-8.403	27.901	15.686	1.00	70.36	B
4306	CD	GLU	B1083	-7.406	27.767	16.899	1.00	67.30	B
4307	OE1	GLU	B1083	-7.785	28.018	18.028	1.00	65.53	B
4308	OE2	GLU	B1083	-6.260	27.304	16.736	1.00	65.12	B
4309	C	GLU	B1083	-6.067	27.943	12.530	1.00	69.34	B
4310	O	GLU	B1083	-5.629	26.857	12.299	1.00	70.77	B
4311	N	VAL	B1084	-6.048	28.981	11.720	1.00	66.88	B
4312	CA	VAL	B1084	-6.001	28.996	10.352	1.00	66.37	B
4313	CB	VAL	B1084	-7.439	28.964	9.883	1.00	67.27	B
4314	CG1	VAL	B1084	-8.172	27.874	10.677	1.00	68.23	B
4315	CG2	VAL	B1084	-8.142	30.333	10.118	1.00	64.32	B
4316	C	VAL	B1084	-5.315	30.377	9.955	1.00	67.14	B
4317	O	VAL	B1084	-5.949	31.447	9.886	1.00	66.68	B
4318	N	PRO	B1085	-4.007	30.323	9.645	1.00	66.33	B
4319	CD	PRO	B1085	-3.316	29.006	9.601	1.00	63.57	B
4320	CA	PRO	B1085	-3.124	31.461	9.363	1.00	65.67	B
4321	CB	PRO	B1085	-2.071	30.816	8.527	1.00	65.31	B
4322	CG	PRO	B1085	-2.056	29.321	9.125	1.00	64.76	B
4323	C	PRO	B1085	-3.605	32.713	8.633	1.00	66.26	B
4324	O	PRO	B1085	-2.943	33.052	7.666	1.00	67.83	B
4325	N	GLY	B1086	-4.635	33.447	9.149	1.00	68.49	B
4326	CA	GLY	B1086	-5.304	34.761	8.643	1.00	66.36	B
4327	C	GLY	B1086	-4.396	35.900	8.283	1.00	68.28	B
4328	O	GLY	B1086	-3.214	35.669	8.027	1.00	69.71	B
4329	N	PRO	B1087	-4.897	37.154	8.178	1.00	68.51	B
4330	CD	PRO	B1087	-6.181	37.763	8.611	1.00	68.98	B
4331	CA	PRO	B1087	-3.998	38.145	7.446	1.00	67.40	B
4332	CB	PRO	B1087	-5.017	39.159	6.857	1.00	67.88	B
4333	CG	PRO	B1087	-6.396	38.972	7.682	1.00	66.71	B
4334	C	PRO	B1087	-3.074	38.881	8.421	1.00	67.03	B
4335	O	PRO	B1087	-1.953	39.342	8.105	1.00	63.67	B
4336	N	ASP	B1088	-3.652	38.974	9.629	1.00	67.76	B
4337	CA	ASP	B1088	-3.139	39.747	10.716	1.00	67.98	B
4338	CB	ASP	B1088	-4.303	40.222	11.596	1.00	68.91	B
4339	CG	ASP	B1088	-4.957	41.565	11.063	1.00	76.04	B
4340	OD1	ASP	B1088	-6.208	41.698	10.867	1.00	79.34	B
4341	OD2	ASP	B1088	-4.199	42.535	10.851	1.00	79.03	B
4342	C	ASP	B1088	-2.202	38.838	11.443	1.00	66.00	B
4343	O	ASP	B1088	-1.981	39.044	12.640	1.00	66.17	B
4344	N	CYS	B1089	-1.656	37.869	10.691	1.00	64.62	B
4345	CA	CYS	B1089	-0.824	36.704	11.187	1.00	64.72	B
4346	CB	CYS	B1089	-1.287	35.358	10.684	1.00	60.77	B
4347	SG	CYS	B1089	-2.826	34.853	11.496	1.00	63.68	B
4348	C	CYS	B1089	0.665	36.742	10.897	1.00	66.26	B
4349	O	CYS	B1089	1.465	36.623	11.851	1.00	69.18	B
4350	N	ARG	B1090	1.059	36.913	9.624	1.00	65.36	B
4351	CA	ARG	B1090	2.460	37.099	9.289	1.00	64.65	B
4352	CB	ARG	B1090	2.565	37.640	7.826	1.00	64.12	B
4353	CG	ARG	B1090	1.489	37.069	6.766	1.00	67.29	B
4354	CD	ARG	B1090	2.011	37.218	5.172	1.00	67.93	B
4355	NE	ARG	B1090	2.430	38.579	4.633	1.00	55.08	B

4356	CZ	ARG	B1090	3.162	38.658	3.563	1.00	59.33	B
4357	NH1	ARG	B1090	3.673	37.484	3.032	1.00	59.93	B
4358	NH2	ARG	B1090	3.442	39.867	3.047	1.00	55.54	B
4359	C	ARG	B1090	3.244	38.009	10.320	1.00	62.38	B
4360	O	ARG	B1090	2.648	38.917	10.944	1.00	63.64	B
4361	N	PHE	B1091	4.551	37.856	10.437	1.00	59.56	B
4362	CA	PHE	B1091	5.337	38.887	11.094	1.00	59.74	B
4363	CB	PHE	B1091	5.604	38.618	12.671	1.00	58.40	B
4364	CG	PHE	B1091	4.314	38.663	13.538	1.00	55.93	B
4365	CD1	PHE	B1091	3.823	39.918	14.019	1.00	54.95	B
4366	CD2	PHE	B1091	3.573	37.521	13.795	1.00	48.46	B
4367	CE1	PHE	B1091	2.624	40.048	14.684	1.00	45.72	B
4368	CE2	PHE	B1091	2.387	37.621	14.481	1.00	47.05	B
4369	CZ	PHE	B1091	1.911	38.917	14.930	1.00	51.42	B
4370	C	PHE	B1091	6.624	38.954	10.325	1.00	58.88	B
4371	O	PHE	B1091	7.035	37.971	9.775	1.00	58.32	B
4372	N	LEU	B1092	7.237	40.121	10.332	1.00	58.29	B
4373	CA	LEU	B1092	8.563	40.312	9.800	1.00	58.12	B
4374	CB	LEU	B1092	8.583	41.465	8.772	1.00	57.50	B
4375	CG	LEU	B1092	7.239	41.467	7.980	1.00	53.91	B
4376	CD1	LEU	B1092	7.057	42.722	7.004	1.00	38.98	B
4377	CD2	LEU	B1092	7.295	40.108	7.296	1.00	39.47	B
4378	C	LEU	B1092	9.644	40.482	10.927	1.00	58.88	B
4379	O	LEU	B1092	10.073	41.595	11.330	1.00	56.19	B
4380	N	ILE	B1093	10.073	39.286	11.366	1.00	58.65	B
4381	CA	ILE	B1093	11.314	39.043	12.099	1.00	54.71	B
4382	CB	ILE	B1093	11.723	37.540	12.129	1.00	51.84	B
4383	CG2	ILE	B1093	12.622	37.266	13.218	1.00	49.87	B
4384	CG1	ILE	B1093	10.607	36.678	12.522	1.00	50.76	B
4385	CD1	ILE	B1093	9.480	37.266	12.147	1.00	50.85	B
4386	C	ILE	B1093	12.434	39.614	11.406	1.00	55.29	B
4387	O	ILE	B1093	13.032	38.900	10.585	1.00	58.10	B
4388	N	VAL	B1094	12.861	40.816	11.725	1.00	55.30	B
4389	CA	VAL	B1094	14.289	40.870	11.435	1.00	57.24	B
4390	CB	VAL	B1094	14.781	41.594	10.056	1.00	57.58	B
4391	CG1	VAL	B1094	16.361	41.586	9.889	1.00	59.29	B
4392	CG2	VAL	B1094	14.045	41.086	8.730	1.00	46.01	B
4393	C	VAL	B1094	15.046	41.201	12.665	1.00	60.36	B
4394	O	VAL	B1094	14.892	42.305	13.182	1.00	64.23	B
4395	N	ALA	B1095	15.836	40.220	13.143	1.00	60.88	B
4396	CA	ALA	B1095	16.791	40.438	14.219	1.00	61.39	B
4397	CB	ALA	B1095	17.694	39.319	14.359	1.00	63.36	B
4398	C	ALA	B1095	17.626	41.540	14.028	1.00	61.00	B
4399	O	ALA	B1095	17.699	41.997	12.960	1.00	61.06	B
4400	N	HIS	B1096	18.313	41.944	15.096	1.00	64.16	B
4401	CA	HIS	B1096	19.461	42.876	14.966	1.00	65.11	B
4402	CB	HIS	B1096	19.259	44.251	15.646	1.00	64.44	B
4403	CG	HIS	B1096	17.842	44.754	15.693	1.00	62.87	B
4404	CD2	HIS	B1096	16.791	44.370	16.437	1.00	63.22	B
4405	ND1	HIS	B1096	17.379	45.779	14.902	1.00	66.64	B
4406	CE1	HIS	B1096	16.119	46.027	15.180	1.00	61.69	B
4407	NE2	HIS	B1096	15.745	45.202	16.122	1.00	61.77	B
4408	C	HIS	B1096	20.869	42.330	15.352	1.00	66.77	B
4409	O	HIS	B1096	21.359	41.267	14.844	1.00	66.14	B
4410	N	ASP	B1097	21.576	43.120	16.167	1.00	68.04	B
4411	CA	ASP	B1097	23.051	43.029	16.065	1.00	68.60	B

4412	CB	ASP	B1097	23.703	44.437	16.185	1.00	69.50	B
4413	CG	ASP	B1097	24.426	44.951	14.869	1.00	68.44	B
4414	OD1	ASP	B1097	23.780	45.127	13.737	1.00	68.44	B
4415	OD2	ASP	B1097	25.662	45.184	15.028	1.00	58.79	B
4416	C	ASP	B1097	23.484	42.053	17.148	1.00	69.20	B
4417	O	ASP	B1097	23.447	40.820	16.944	1.00	71.01	B
4418	N	ASP	B1098	23.870	42.603	18.306	1.00	69.14	B
4419	CA	ASP	B1098	23.835	41.929	19.600	1.00	67.30	B
4420	CB	ASP	B1098	24.992	42.479	20.489	1.00	67.87	B
4421	CG	ASP	B1098	26.318	42.841	19.670	1.00	62.96	B
4422	OD1	ASP	B1098	26.348	43.763	18.805	1.00	66.36	B
4423	OD2	ASP	B1098	27.362	42.278	19.954	1.00	55.30	B
4424	C	ASP	B1098	22.459	42.413	20.124	1.00	66.51	B
4425	O	ASP	B1098	22.333	42.859	21.280	1.00	64.78	B
4426	N	GLY	B1099	21.463	42.352	19.210	1.00	65.78	B
4427	CA	GLY	B1099	20.261	43.250	19.188	1.00	64.86	B
4428	C	GLY	B1099	19.357	42.200	19.620	1.00	63.59	B
4429	O	GLY	B1099	19.903	41.340	20.301	1.00	65.27	B
4430	N	ARG	B1100	18.092	42.135	19.172	1.00	61.64	B
4431	CA	ARG	B1100	17.346	40.865	19.366	1.00	62.00	B
4432	CB	ARG	B1100	16.746	40.624	20.811	1.00	64.43	B
4433	CG	ARG	B1100	17.702	39.939	21.887	1.00	57.71	B
4434	CD	ARG	B1100	18.369	41.093	22.505	1.00	63.49	B
4435	NE	ARG	B1100	17.529	42.318	22.606	1.00	54.85	B
4436	CZ	ARG	B1100	18.046	43.498	22.861	1.00	63.24	B
4437	NH1	ARG	B1100	19.392	43.528	22.955	1.00	60.99	B
4438	NH2	ARG	B1100	17.245	44.631	22.968	1.00	67.53	B
4439	C	ARG	B1100	16.423	40.440	18.208	1.00	61.11	B
4440	O	ARG	B1100	16.947	40.562	17.124	1.00	61.67	B
4441	N	TRP	B1101	15.211	39.841	18.417	1.00	56.85	B
4442	CA	TRP	B1101	14.232	39.787	17.330	1.00	56.52	B
4443	CB	TRP	B1101	13.377	38.473	17.136	1.00	53.72	B
4444	CG	TRP	B1101	13.941	37.347	16.560	1.00	52.04	B
4445	CD2	TRP	B1101	13.332	36.069	16.416	1.00	50.51	B
4446	CE2	TRP	B1101	14.285	35.203	15.750	1.00	50.88	B
4447	CE3	TRP	B1101	12.040	35.575	16.673	1.00	52.27	B
4448	CD1	TRP	B1101	15.246	37.217	16.048	1.00	55.64	B
4449	NE1	TRP	B1101	15.411	35.936	15.484	1.00	54.85	B
4450	CZ2	TRP	B1101	13.994	33.895	15.411	1.00	49.64	B
4451	CZ3	TRP	B1101	11.714	34.281	16.295	1.00	48.05	B
4452	CH2	TRP	B1101	12.692	33.447	15.669	1.00	52.95	B
4453	C	TRP	B1101	13.209	40.927	17.525	1.00	58.87	B
4454	O	TRP	B1101	13.143	41.509	18.566	1.00	61.49	B
4455	N	SER	B1102	12.291	41.126	16.589	1.00	58.46	B
4456	CA	SER	B1102	11.606	42.304	16.622	1.00	58.61	B
4457	CB	SER	B1102	12.515	43.441	16.103	1.00	58.81	B
4458	OG	SER	B1102	11.938	44.744	16.221	1.00	58.65	B
4459	C	SER	B1102	10.683	41.908	15.581	1.00	58.25	B
4460	O	SER	B1102	11.019	42.042	14.511	1.00	56.88	B
4461	N	LEU	B1103	9.527	41.387	15.975	1.00	59.97	B
4462	CA	LEU	B1103	8.417	41.037	15.137	1.00	59.12	B
4463	CB	LEU	B1103	7.506	40.053	15.830	1.00	59.24	B
4464	CG	LEU	B1103	8.127	38.799	16.509	1.00	61.64	B
4465	CD1	LEU	B1103	8.804	37.865	15.464	1.00	64.77	B
4466	CD2	LEU	B1103	9.185	39.178	17.695	1.00	58.21	B
4467	C	LEU	B1103	7.649	42.257	14.883	1.00	58.65	B

4468	O	LEU	B1103	7.352	42.996	15.834	1.00	60.08	B
4469	N	GLN	B1104	7.321	42.432	13.585	1.00	56.90	B
4470	CA	GLN	B1104	6.638	43.532	13.038	1.00	53.95	B
4471	CB	GLN	B1104	7.680	44.312	12.351	1.00	50.13	B
4472	CG	GLN	B1104	6.976	45.473	11.825	1.00	55.40	B
4473	CD	GLN	B1104	7.262	46.020	10.333	1.00	46.76	B
4474	OE1	GLN	B1104	7.541	45.296	9.426	1.00	41.63	B
4475	NE2	GLN	B1104	7.076	47.341	10.172	1.00	42.70	B
4476	C	GLN	B1104	5.484	43.078	12.056	1.00	55.86	B
4477	O	GLN	B1104	5.721	42.550	10.961	1.00	60.32	B
4478	N	SER	B1105	4.235	43.293	12.404	1.00	55.28	B
4479	CA	SER	B1105	3.099	42.825	11.654	1.00	55.14	B
4480	CB	SER	B1105	1.876	43.587	12.141	1.00	53.88	B
4481	OG	SER	B1105	2.202	44.972	12.381	1.00	55.74	B
4482	C	SER	B1105	3.217	43.077	10.178	1.00	56.75	B
4483	O	SER	B1105	3.636	44.211	9.880	1.00	59.75	B
4484	N	GLU	B1106	2.870	42.122	9.250	1.00	56.54	B
4485	CA	GLU	B1106	3.198	42.401	7.845	1.00	56.95	B
4486	CB	GLU	B1106	3.654	41.211	6.898	1.00	57.24	B
4487	CG	GLU	B1106	3.923	41.720	5.361	1.00	57.17	B
4488	CD	GLU	B1106	5.262	41.238	4.687	1.00	60.81	B
4489	OE1	GLU	B1106	5.507	39.997	4.626	1.00	54.56	B
4490	OE2	GLU	B1106	6.082	42.091	4.162	1.00	59.37	B
4491	C	GLU	B1106	2.387	43.555	7.183	1.00	55.43	B
4492	O	GLU	B1106	2.966	44.553	6.799	1.00	53.46	B
4493	N	ALA	B1107	1.103	43.332	7.000	1.00	54.76	B
4494	CA	ALA	B1107	0.154	44.415	6.847	1.00	56.78	B
4495	CB	ALA	B1107	-1.246	43.892	7.082	1.00	54.26	B
4496	C	ALA	B1107	0.453	45.583	7.896	1.00	58.38	B
4497	O	ALA	B1107	1.159	46.668	7.627	1.00	59.21	B
4498	N	HIS	B1108	-0.125	45.418	9.067	1.00	55.86	B
4499	CA	HIS	B1108	-0.201	46.572	9.847	1.00	55.47	B
4500	CB	HIS	B1108	-0.961	46.210	11.010	1.00	55.70	B
4501	CG	HIS	B1108	-2.250	45.547	10.601	1.00	54.81	B
4502	CD2	HIS	B1108	-2.956	44.523	11.131	1.00	55.20	B
4503	ND1	HIS	B1108	-3.009	46.008	9.548	1.00	53.03	B
4504	CE1	HIS	B1108	-4.115	45.278	9.416	1.00	44.92	B
4505	NE2	HIS	B1108	-4.117	44.385	10.384	1.00	51.22	B
4506	C	HIS	B1108	1.046	47.409	9.839	1.00	55.85	B
4507	O	HIS	B1108	0.925	48.297	9.045	1.00	57.62	B
4508	N	ARG	B1109	2.248	47.028	10.409	1.00	56.47	B
4509	CA	ARG	B1109	3.583	47.749	10.372	1.00	57.18	B
4510	CB	ARG	B1109	3.443	49.039	9.643	1.00	57.10	B
4511	CG	ARG	B1109	4.760	49.796	9.195	1.00	57.51	B
4512	CD	ARG	B1109	5.091	49.677	7.700	1.00	49.48	B
4513	NE	ARG	B1109	5.382	48.216	7.449	1.00	51.37	B
4514	CZ	ARG	B1109	4.458	47.283	7.225	1.00	42.77	B
4515	NH1	ARG	B1109	3.136	47.704	7.202	1.00	27.90	B
4516	NH2	ARG	B1109	4.911	46.000	6.964	1.00	31.24	B
4517	C	ARG	B1109	3.990	48.056	11.824	1.00	61.38	B
4518	O	ARG	B1109	4.985	48.752	12.206	1.00	60.72	B
4519	N	ARG	B1110	3.184	47.423	12.657	1.00	62.26	B
4520	CA	ARG	B1110	3.231	47.556	14.063	1.00	62.81	B
4521	CB	ARG	B1110	1.747	47.429	14.547	1.00	62.09	B
4522	CG	ARG	B1110	0.696	48.465	13.933	1.00	63.18	B
4523	CD	ARG	B1110	0.388	49.677	14.699	1.00	51.87	B

4524	NE	ARG	B1110	0.905	50.855	14.094	1.00	51.84	B
4525	CZ	ARG	B1110	0.407	52.085	14.248	1.00	59.87	B
4526	NH1	ARG	B1110	-0.687	52.294	14.995	1.00	63.89	B
4527	NH2	ARG	B1110	0.938	53.129	13.590	1.00	65.78	B
4528	C	ARG	B1110	4.165	46.498	14.862	1.00	62.60	B
4529	O	ARG	B1110	3.961	45.290	14.809	1.00	57.87	B
4530	N	TYR	B1111	5.068	47.030	15.720	1.00	63.48	B
4531	CA	TYR	B1111	6.014	46.212	16.503	1.00	61.64	B
4532	CB	TYR	B1111	7.192	47.041	16.895	1.00	60.26	B
4533	CG	TYR	B1111	8.003	47.471	15.685	1.00	63.00	B
4534	CD1	TYR	B1111	7.684	48.607	14.961	1.00	65.07	B
4535	CE1	TYR	B1111	8.440	49.003	13.766	1.00	61.15	B
4536	CD2	TYR	B1111	9.064	46.700	15.192	1.00	63.67	B
4537	CE2	TYR	B1111	9.841	47.134	13.991	1.00	60.98	B
4538	CZ	TYR	B1111	9.483	48.258	13.289	1.00	60.51	B
4539	OH	TYR	B1111	10.206	48.677	12.142	1.00	62.40	B
4540	C	TYR	B1111	5.295	45.618	17.630	1.00	61.29	B
4541	O	TYR	B1111	4.697	46.306	18.454	1.00	62.62	B
4542	N	PHE	B1112	5.238	44.294	17.583	1.00	60.83	B
4543	CA	PHE	B1112	4.910	43.462	18.735	1.00	58.41	B
4544	CB	PHE	B1112	5.099	42.006	18.330	1.00	58.40	B
4545	CG	PHE	B1112	4.792	41.026	19.392	1.00	52.91	B
4546	CD1	PHE	B1112	3.518	40.881	19.841	1.00	49.62	B
4547	CD2	PHE	B1112	5.771	40.203	19.878	1.00	56.05	B
4548	CE1	PHE	B1112	3.153	39.955	20.823	1.00	47.42	B
4549	CE2	PHE	B1112	5.454	39.154	20.869	1.00	52.19	B
4550	CZ	PHE	B1112	4.113	39.066	21.346	1.00	51.38	B
4551	C	PHE	B1112	5.902	43.767	19.842	1.00	58.33	B
4552	O	PHE	B1112	7.161	43.793	19.717	1.00	57.25	B
4553	N	GLY	B1113	5.351	44.037	20.961	1.00	58.52	B
4554	CA	GLY	B1113	6.283	44.219	22.028	1.00	57.43	B
4555	C	GLY	B1113	5.755	44.221	23.400	1.00	55.34	B
4556	O	GLY	B1113	6.497	44.495	24.177	1.00	57.64	B
4557	N	GLY	B1114	4.556	43.783	23.716	1.00	55.29	B
4558	CA	GLY	B1114	3.960	44.000	25.088	1.00	57.08	B
4559	C	GLY	B1114	4.688	43.860	26.468	1.00	55.49	B
4560	O	GLY	B1114	5.623	44.592	26.654	1.00	55.67	B
4561	N	THR	B1115	4.289	42.909	27.375	1.00	55.33	B
4562	CA	THR	B1115	4.808	42.785	28.855	1.00	53.54	B
4563	CB	THR	B1115	5.049	44.194	29.546	1.00	53.46	B
4564	OG1	THR	B1115	6.452	44.519	29.738	1.00	52.93	B
4565	CG2	THR	B1115	4.182	44.440	30.776	1.00	49.59	B
4566	C	THR	B1115	3.721	42.047	29.639	1.00	53.08	B
4567	O	THR	B1115	2.484	42.446	29.624	1.00	48.68	B
4568	N	GLU	B1116	4.137	40.969	30.322	1.00	54.81	B
4569	CA	GLU	B1116	3.233	40.305	31.293	1.00	55.17	B
4570	CB	GLU	B1116	3.031	41.208	32.560	1.00	53.98	B
4571	CG	GLU	B1116	2.651	40.636	33.837	1.00	50.78	B
4572	CD	GLU	B1116	2.643	39.101	33.881	1.00	58.26	B
4573	OE1	GLU	B1116	1.647	38.590	34.421	1.00	64.55	B
4574	OE2	GLU	B1116	3.565	38.383	33.414	1.00	54.32	B
4575	C	GLU	B1116	2.001	40.267	30.554	1.00	56.92	B
4576	O	GLU	B1116	1.915	39.594	29.489	1.00	62.55	B
4577	N	ASP	B1117	1.047	41.024	30.988	1.00	56.14	B
4578	CA	ASP	B1117	-0.287	40.703	30.513	1.00	57.48	B
4579	CB	ASP	B1117	-0.961	40.648	31.862	1.00	57.01	B

4580	CG	ASP	B1117	-1.812	41.865	32.132	1.00	51.07	B
4581	OD1	ASP	B1117	-1.380	43.035	31.879	1.00	46.51	B
4582	OD2	ASP	B1117	-2.920	41.536	32.591	1.00	45.46	B
4583	C	ASP	B1117	-1.102	41.704	29.459	1.00	57.40	B
4584	O	ASP	B1117	-2.312	41.634	29.262	1.00	53.01	B
4585	N	ARG	B1118	-0.393	42.673	28.875	1.00	59.77	B
4586	CA	ARG	B1118	-0.961	43.858	28.209	1.00	61.30	B
4587	CB	ARG	B1118	-1.103	45.001	29.265	1.00	60.09	B
4588	CG	ARG	B1118	-0.832	46.503	28.819	1.00	69.19	B
4589	CD	ARG	B1118	-1.997	47.656	29.363	1.00	67.69	B
4590	NE	ARG	B1118	-3.299	46.994	29.611	1.00	82.13	B
4591	CZ	ARG	B1118	-4.097	46.417	28.663	1.00	88.78	B
4592	NH1	ARG	B1118	-3.779	46.386	27.331	1.00	91.32	B
4593	NH2	ARG	B1118	-5.256	45.841	29.034	1.00	92.47	B
4594	C	ARG	B1118	0.005	44.205	27.044	1.00	61.72	B
4595	O	ARG	B1118	0.391	45.439	26.912	1.00	62.81	B
4596	N	LEU	B1119	0.382	43.145	26.237	1.00	60.76	B
4597	CA	LEU	B1119	1.103	43.221	24.854	1.00	60.81	B
4598	CB	LEU	B1119	1.709	41.915	24.369	1.00	59.74	B
4599	CG	LEU	B1119	2.151	40.720	25.247	1.00	63.06	B
4600	CD1	LEU	B1119	1.136	40.131	26.261	1.00	61.58	B
4601	CD2	LEU	B1119	2.403	39.649	24.208	1.00	62.02	B
4602	C	LEU	B1119	0.241	43.641	23.632	1.00	59.08	B
4603	O	LEU	B1119	-0.908	43.174	23.477	1.00	54.29	B
4604	N	SER	B1120	0.824	44.570	22.863	1.00	58.36	B
4605	CA	SER	B1120	0.201	45.127	21.681	1.00	57.61	B
4606	CB	SER	B1120	-0.097	46.603	21.962	1.00	58.09	B
4607	OG	SER	B1120	0.994	47.435	21.557	1.00	56.33	B
4608	C	SER	B1120	1.066	45.073	20.443	1.00	56.27	B
4609	O	SER	B1120	2.249	45.156	20.520	1.00	55.86	B
4610	N	CYS	B1121	0.489	45.022	19.269	1.00	57.53	B
4611	CA	CYS	B1121	1.332	45.348	18.061	1.00	58.85	B
4612	CB	CYS	B1121	0.921	44.533	16.787	1.00	58.16	B
4613	SG	CYS	B1121	2.355	43.884	15.785	1.00	61.16	B
4614	C	CYS	B1121	1.190	46.803	17.688	1.00	57.96	B
4615	O	CYS	B1121	0.430	47.048	16.757	1.00	59.24	B
4616	N	PHE	B1122	1.750	47.773	18.403	1.00	56.13	B
4617	CA	PHE	B1122	1.300	49.110	18.051	1.00	55.70	B
4618	CB	PHE	B1122	0.394	49.733	19.070	1.00	58.52	B
4619	CG	PHE	B1122	-0.642	50.812	18.480	1.00	60.08	B
4620	CD1	PHE	B1122	-0.325	52.208	18.495	1.00	61.43	B
4621	CD2	PHE	B1122	-1.944	50.419	18.039	1.00	58.13	B
4622	CE1	PHE	B1122	-1.218	53.148	18.035	1.00	61.52	B
4623	CE2	PHE	B1122	-2.883	51.354	17.630	1.00	56.99	B
4624	CZ	PHE	B1122	-2.504	52.750	17.575	1.00	58.94	B
4625	C	PHE	B1122	2.272	50.078	17.818	1.00	54.64	B
4626	O	PHE	B1122	1.895	51.070	17.332	1.00	56.54	B
4627	N	ALA	B1123	3.511	49.725	18.022	1.00	53.81	B
4628	CA	ALA	B1123	4.602	50.599	18.357	1.00	54.89	B
4629	CB	ALA	B1123	5.536	49.913	19.342	1.00	48.73	B
4630	C	ALA	B1123	5.283	50.780	17.026	1.00	56.46	B
4631	O	ALA	B1123	5.707	49.752	16.403	1.00	57.75	B
4632	N	GLN	B1124	5.410	52.053	16.621	1.00	56.05	B
4633	CA	GLN	B1124	5.692	52.382	15.301	1.00	56.80	B
4634	CB	GLN	B1124	4.747	53.461	14.811	1.00	55.61	B
4635	CG	GLN	B1124	5.043	54.864	15.069	1.00	56.02	B

4636	CD	GLN	B1124	3.853	55.784	14.613	1.00	56.43	B
4637	OE1	GLN	B1124	2.737	55.283	14.279	1.00	62.23	B
4638	NE2	GLN	B1124	4.085	57.097	14.549	1.00	48.49	B
4639	C	GLN	B1124	7.172	52.599	15.223	1.00	59.22	B
4640	O	GLN	B1124	7.786	53.234	14.324	1.00	60.29	B
4641	N	THR	B1125	7.805	52.007	16.221	1.00	61.63	B
4642	CA	THR	B1125	9.300	52.113	16.403	1.00	61.49	B
4643	CB	THR	B1125	9.641	53.583	16.672	1.00	57.41	B
4644	OG1	THR	B1125	10.752	53.656	17.502	1.00	57.92	B
4645	CG2	THR	B1125	8.572	54.153	17.498	1.00	64.08	B
4646	C	THR	B1125	9.803	50.985	17.461	1.00	61.88	B
4647	O	THR	B1125	9.163	50.679	18.463	1.00	60.06	B
4648	N	VAL	B1126	10.896	50.296	17.178	1.00	64.31	B
4649	CA	VAL	B1126	11.458	49.325	18.141	1.00	64.90	B
4650	CB	VAL	B1126	12.822	48.694	17.673	1.00	66.92	B
4651	CG1	VAL	B1126	12.752	48.092	16.302	1.00	64.65	B
4652	CG2	VAL	B1126	14.055	49.772	17.908	1.00	68.80	B
4653	C	VAL	B1126	11.788	50.123	19.439	1.00	65.08	B
4654	O	VAL	B1126	11.307	51.285	19.549	1.00	67.17	B
4655	N	SER	B1127	12.629	49.564	20.363	1.00	61.30	B
4656	CA	SER	B1127	12.516	50.001	21.744	1.00	56.72	B
4657	CB	SER	B1127	11.148	50.559	21.930	1.00	54.62	B
4658	OG	SER	B1127	11.299	51.676	22.658	1.00	47.51	B
4659	C	SER	B1127	12.540	48.766	22.635	1.00	57.82	B
4660	O	SER	B1127	11.691	47.811	22.429	1.00	55.72	B
4661	N	PRO	B1128	13.430	48.820	23.667	1.00	55.95	B
4662	CD	PRO	B1128	14.064	50.105	23.943	1.00	57.65	B
4663	CA	PRO	B1128	13.701	47.963	24.682	1.00	55.35	B
4664	CB	PRO	B1128	13.944	48.910	25.874	1.00	56.36	B
4665	CG	PRO	B1128	13.589	50.374	25.380	1.00	56.13	B
4666	C	PRO	B1128	12.403	47.312	24.895	1.00	57.12	B
4667	O	PRO	B1128	12.360	46.133	24.901	1.00	59.52	B
4668	N	ALA	B1129	11.301	48.024	25.046	1.00	57.55	B
4669	CA	ALA	B1129	10.015	47.346	25.364	1.00	58.55	B
4670	CB	ALA	B1129	8.912	48.349	25.527	1.00	56.68	B
4671	C	ALA	B1129	9.590	46.211	24.399	1.00	59.79	B
4672	O	ALA	B1129	9.012	45.148	24.846	1.00	60.88	B
4673	N	GLU	B1130	9.940	46.434	23.117	1.00	60.84	B
4674	CA	GLU	B1130	9.565	45.576	21.957	1.00	62.09	B
4675	CB	GLU	B1130	9.232	46.344	20.607	1.00	62.04	B
4676	CG	GLU	B1130	8.936	47.867	20.497	1.00	60.88	B
4677	CD	GLU	B1130	8.217	48.659	21.652	1.00	54.30	B
4678	OE1	GLU	B1130	8.838	49.683	22.081	1.00	55.94	B
4679	OE2	GLU	B1130	7.072	48.363	22.050	1.00	51.60	B
4680	C	GLU	B1130	10.588	44.485	21.550	1.00	61.90	B
4681	O	GLU	B1130	10.288	43.762	20.644	1.00	62.09	B
4682	N	LYS	B1131	11.756	44.428	22.225	1.00	62.20	B
4683	CA	LYS	B1131	12.969	43.638	21.950	1.00	61.03	B
4684	CB	LYS	B1131	14.129	44.328	22.684	1.00	60.07	B
4685	CG	LYS	B1131	14.598	45.594	22.107	1.00	61.44	B
4686	CD	LYS	B1131	14.769	45.466	20.441	1.00	62.70	B
4687	CE	LYS	B1131	15.909	46.321	19.838	1.00	56.46	B
4688	NZ	LYS	B1131	17.393	46.015	19.785	1.00	54.36	B
4689	C	LYS	B1131	12.836	42.199	22.459	1.00	61.35	B
4690	O	LYS	B1131	12.733	41.896	23.665	1.00	60.12	B
4691	N	TRP	B1132	12.803	41.253	21.564	1.00	61.88	B

4692	CA	TRP	B1132	12.424	39.919	22.111	1.00	61.77	B
4693	CB	TRP	B1132	11.359	39.438	21.295	1.00	56.95	B
4694	CG	TRP	B1132	10.241	40.247	21.583	1.00	56.83	B
4695	CD2	TRP	B1132	9.292	39.992	22.635	1.00	52.56	B
4696	CE2	TRP	B1132	8.309	41.002	22.577	1.00	44.07	B
4697	CE3	TRP	B1132	9.174	38.995	23.575	1.00	45.92	B
4698	CD1	TRP	B1132	9.882	41.422	20.991	1.00	47.76	B
4699	NE1	TRP	B1132	8.667	41.876	21.589	1.00	48.76	B
4700	CZ2	TRP	B1132	7.311	41.042	23.403	1.00	45.87	B
4701	CZ3	TRP	B1132	8.172	39.042	24.355	1.00	51.15	B
4702	CH2	TRP	B1132	7.245	40.048	24.294	1.00	50.90	B
4703	C	TRP	B1132	13.402	38.834	22.019	1.00	63.25	B
4704	O	TRP	B1132	13.506	38.288	20.870	1.00	64.60	B
4705	N	SER	B1133	14.165	38.612	23.142	1.00	63.39	B
4706	CA	SER	B1133	15.370	37.639	23.246	1.00	61.80	B
4707	CB	SER	B1133	15.845	37.518	24.764	1.00	62.44	B
4708	OG	SER	B1133	17.244	37.666	25.003	1.00	54.69	B
4709	C	SER	B1133	14.769	36.332	22.730	1.00	61.63	B
4710	O	SER	B1133	13.512	36.073	22.987	1.00	62.00	B
4711	N	VAL	B1134	15.536	35.605	21.921	1.00	59.23	B
4712	CA	VAL	B1134	15.096	34.282	21.389	1.00	60.77	B
4713	CB	VAL	B1134	15.593	34.179	19.946	1.00	61.56	B
4714	CG1	VAL	B1134	15.202	32.836	19.383	1.00	62.56	B
4715	CG2	VAL	B1134	14.973	35.254	19.073	1.00	63.04	B
4716	C	VAL	B1134	15.629	32.955	22.087	1.00	60.93	B
4717	O	VAL	B1134	16.827	32.676	22.006	1.00	58.96	B
4718	N	HIS	B1135	14.805	32.159	22.821	1.00	63.08	B
4719	CA	HIS	B1135	15.309	30.838	23.393	1.00	62.48	B
4720	CB	HIS	B1135	14.916	30.486	24.792	1.00	59.25	B
4721	CG	HIS	B1135	16.105	30.123	25.616	1.00	63.80	B
4722	CD2	HIS	B1135	16.785	28.954	25.741	1.00	66.22	B
4723	ND1	HIS	B1135	16.878	31.070	26.296	1.00	65.45	B
4724	CE1	HIS	B1135	17.920	30.488	26.881	1.00	62.70	B
4725	NE2	HIS	B1135	17.899	29.203	26.540	1.00	65.56	B
4726	C	HIS	B1135	14.786	29.874	22.401	1.00	65.48	B
4727	O	HIS	B1135	13.484	29.831	22.218	1.00	66.14	B
4728	N	ILE	B1136	15.713	29.293	21.576	1.00	65.18	B
4729	CA	ILE	B1136	15.187	28.499	20.417	1.00	64.63	B
4730	CB	ILE	B1136	16.001	28.460	19.123	1.00	65.99	B
4731	CG2	ILE	B1136	15.629	27.189	18.457	1.00	71.25	B
4732	CG1	ILE	B1136	15.480	29.456	18.084	1.00	67.67	B
4733	CD1	ILE	B1136	16.328	29.569	16.744	1.00	59.58	B
4734	C	ILE	B1136	15.364	27.185	20.966	1.00	62.46	B
4735	O	ILE	B1136	16.414	26.953	21.541	1.00	64.20	B
4736	N	ALA	B1137	14.368	26.340	20.750	1.00	59.96	B
4737	CA	ALA	B1137	14.252	25.125	21.473	1.00	58.34	B
4738	CB	ALA	B1137	13.230	25.236	22.391	1.00	56.02	B
4739	C	ALA	B1137	13.950	24.081	20.500	1.00	59.79	B
4740	O	ALA	B1137	12.887	23.489	20.552	1.00	60.32	B
4741	N	MET	B1138	14.871	23.867	19.547	1.00	62.18	B
4742	CA	MET	B1138	14.799	22.715	18.621	1.00	63.70	B
4743	CB	MET	B1138	13.936	22.926	17.390	1.00	64.40	B
4744	CG	MET	B1138	14.554	23.986	16.417	1.00	68.33	B
4745	SD	MET	B1138	13.607	25.483	15.775	1.00	67.45	B
4746	CE	MET	B1138	15.165	26.343	15.370	1.00	66.79	B
4747	C	MET	B1138	16.223	22.447	18.273	1.00	63.11	B

4748	O	MET	B1138	17.164	23.184	18.728	1.00	60.87	B
4749	N	HIS	B1139	16.376	21.352	17.524	1.00	61.38	B
4750	CA	HIS	B1139	17.545	20.525	17.652	1.00	59.71	B
4751	CB	HIS	B1139	17.065	19.040	17.575	1.00	59.49	B
4752	CG	HIS	B1139	18.142	17.986	17.600	1.00	57.77	B
4753	CD2	HIS	B1139	18.182	16.827	18.302	1.00	44.62	B
4754	ND1	HIS	B1139	19.317	18.026	16.819	1.00	59.84	B
4755	CE1	HIS	B1139	20.034	16.943	17.095	1.00	53.97	B
4756	NE2	HIS	B1139	19.370	16.216	17.999	1.00	45.49	B
4757	C	HIS	B1139	18.666	21.003	16.628	1.00	60.77	B
4758	O	HIS	B1139	18.689	20.807	15.462	1.00	60.56	B
4759	N	PRO	B1140	19.718	21.540	17.155	1.00	61.79	B
4760	CD	PRO	B1140	20.021	21.291	18.579	1.00	62.24	B
4761	CA	PRO	B1140	20.809	22.167	16.473	1.00	61.05	B
4762	CB	PRO	B1140	21.939	21.894	17.441	1.00	61.98	B
4763	CG	PRO	B1140	21.334	20.778	18.480	1.00	60.14	B
4764	C	PRO	B1140	21.172	21.432	15.186	1.00	61.54	B
4765	O	PRO	B1140	21.664	22.017	14.175	1.00	59.47	B
4766	N	GLN	B1141	21.050	20.108	15.265	1.00	61.90	B
4767	CA	GLN	B1141	21.728	19.377	14.192	1.00	60.97	B
4768	CB	GLN	B1141	22.260	18.020	14.642	1.00	61.23	B
4769	CG	GLN	B1141	23.520	18.142	15.537	1.00	62.58	B
4770	CD	GLN	B1141	23.893	16.770	16.148	1.00	64.02	B
4771	OE1	GLN	B1141	24.694	16.658	17.114	1.00	63.81	B
4772	NE2	GLN	B1141	23.310	15.709	15.570	1.00	57.36	B
4773	C	GLN	B1141	20.650	19.312	13.173	1.00	57.38	B
4774	O	GLN	B1141	19.491	18.991	13.556	1.00	55.16	B
4775	N	VAL	B1142	21.022	19.732	11.952	1.00	52.38	B
4776	CA	VAL	B1142	20.124	19.871	10.885	1.00	50.13	B
4777	CB	VAL	B1142	19.520	21.268	10.936	1.00	49.58	B
4778	CG1	VAL	B1142	18.747	21.429	12.237	1.00	47.82	B
4779	CG2	VAL	B1142	20.526	22.354	10.759	1.00	48.71	B
4780	C	VAL	B1142	21.067	19.652	9.812	1.00	51.77	B
4781	O	VAL	B1142	22.178	19.769	10.138	1.00	55.26	B
4782	N	ASN	B1143	20.721	19.205	8.599	1.00	52.69	B
4783	CA	ASN	B1143	21.507	19.485	7.384	1.00	50.91	B
4784	CB	ASN	B1143	20.969	18.619	6.281	1.00	50.34	B
4785	CG	ASN	B1143	21.645	17.370	6.145	1.00	53.45	B
4786	OD1	ASN	B1143	21.606	16.762	5.095	1.00	50.95	B
4787	ND2	ASN	B1143	22.406	16.986	7.185	1.00	64.92	B
4788	C	ASN	B1143	21.226	20.944	6.832	1.00	52.44	B
4789	O	ASN	B1143	20.249	21.589	7.249	1.00	49.33	B
4790	N	ILE	B1144	22.017	21.370	5.787	1.00	52.91	B
4791	CA	ILE	B1144	21.897	22.641	5.070	1.00	50.94	B
4792	CB	ILE	B1144	22.936	23.652	5.676	1.00	53.76	B
4793	CG2	ILE	B1144	23.021	25.068	4.900	1.00	50.93	B
4794	CG1	ILE	B1144	22.426	24.096	7.085	1.00	50.20	B
4795	CD1	ILE	B1144	23.210	25.253	7.526	1.00	41.86	B
4796	C	ILE	B1144	21.948	22.583	3.587	1.00	50.90	B
4797	O	ILE	B1144	22.759	21.963	3.051	1.00	46.18	B
4798	N	TYR	B1145	20.988	23.215	2.916	1.00	56.07	B
4799	CA	TYR	B1145	20.718	22.992	1.441	1.00	58.11	B
4800	CB	TYR	B1145	19.700	21.835	1.235	1.00	56.68	B
4801	CG	TYR	B1145	19.119	21.718	-0.258	1.00	59.62	B
4802	CD1	TYR	B1145	19.821	20.949	-1.236	1.00	58.76	B
4803	CE1	TYR	B1145	19.422	20.896	-2.620	1.00	59.07	B

4804	CD2	TYR	B1145	17.894	22.405	-0.693	1.00	55.32	B
4805	CE2	TYR	B1145	17.479	22.314	-2.029	1.00	54.07	B
4806	CZ	TYR	B1145	18.252	21.567	-3.021	1.00	59.67	B
4807	OH	TYR	B1145	17.915	21.416	-4.416	1.00	54.79	B
4808	C	TYR	B1145	20.152	24.270	0.712	1.00	60.40	B
4809	O	TYR	B1145	19.004	24.741	1.065	1.00	61.44	B
4810	N	SER	B1146	20.884	24.833	-0.283	1.00	62.03	B
4811	CA	SER	B1146	20.356	26.052	-1.037	1.00	63.22	B
4812	CB	SER	B1146	21.144	27.384	-0.702	1.00	65.08	B
4813	OG	SER	B1146	20.947	27.840	0.685	1.00	64.42	B
4814	C	SER	B1146	20.032	25.862	-2.562	1.00	63.73	B
4815	O	SER	B1146	20.766	25.199	-3.263	1.00	65.89	B
4816	N	VAL	B1147	18.963	26.442	-3.086	1.00	63.15	B
4817	CA	VAL	B1147	18.670	26.267	-4.526	1.00	63.23	B
4818	CB	VAL	B1147	17.213	26.653	-4.773	1.00	63.38	B
4819	CG1	VAL	B1147	16.937	27.258	-6.156	1.00	61.13	B
4820	CG2	VAL	B1147	16.232	25.427	-4.382	1.00	65.27	B
4821	C	VAL	B1147	19.595	27.207	-5.255	1.00	64.27	B
4822	O	VAL	B1147	20.068	26.966	-6.447	1.00	63.13	B
4823	N	THR	B1148	19.877	28.292	-4.515	1.00	64.92	B
4824	CA	THR	B1148	20.955	29.176	-4.926	1.00	66.58	B
4825	CB	THR	B1148	21.145	30.438	-3.889	1.00	67.44	B
4826	OG1	THR	B1148	19.918	31.240	-3.860	1.00	68.55	B
4827	CG2	THR	B1148	22.246	31.482	-4.345	1.00	65.23	B
4828	C	THR	B1148	22.146	28.217	-5.366	1.00	65.87	B
4829	O	THR	B1148	22.484	27.982	-6.557	1.00	67.41	B
4830	N	ARG	B1149	22.640	27.506	-4.418	1.00	64.59	B
4831	CA	ARG	B1149	23.613	26.532	-4.730	1.00	63.02	B
4832	CB	ARG	B1149	24.478	26.316	-3.483	1.00	62.83	B
4833	CG	ARG	B1149	25.729	27.267	-3.502	1.00	56.37	B
4834	CD	ARG	B1149	26.950	26.395	-4.129	1.00	58.52	B
4835	NE	ARG	B1149	28.096	27.284	-4.437	1.00	57.19	B
4836	CZ	ARG	B1149	27.965	28.602	-4.472	1.00	55.88	B
4837	NH1	ARG	B1149	26.733	29.168	-4.193	1.00	50.52	B
4838	NH2	ARG	B1149	29.024	29.302	-4.809	1.00	57.08	B
4839	C	ARG	B1149	23.032	25.238	-5.295	1.00	64.29	B
4840	O	ARG	B1149	23.674	24.607	-6.174	1.00	64.81	B
4841	N	LYS	B1150	21.847	24.810	-4.847	1.00	64.52	B
4842	CA	LYS	B1150	21.120	23.741	-5.577	1.00	64.58	B
4843	CB	LYS	B1150	21.319	23.856	-7.134	1.00	66.67	B
4844	CG	LYS	B1150	20.200	24.642	-7.944	1.00	69.65	B
4845	CD	LYS	B1150	19.189	23.602	-8.590	1.00	77.96	B
4846	CE	LYS	B1150	18.198	22.721	-7.546	1.00	76.91	B
4847	NZ	LYS	B1150	16.734	22.442	-7.983	1.00	67.36	B
4848	C	LYS	B1150	21.583	22.377	-5.091	1.00	63.51	B
4849	O	LYS	B1150	20.807	21.361	-5.159	1.00	65.74	B
4850	N	ARG	B1151	22.780	22.369	-4.522	1.00	59.06	B
4851	CA	ARG	B1151	23.465	21.175	-4.116	1.00	56.59	B
4852	CB	ARG	B1151	24.835	21.224	-4.641	1.00	54.87	B
4853	CG	ARG	B1151	25.039	20.469	-5.691	1.00	50.26	B
4854	CD	ARG	B1151	26.363	20.804	-5.920	1.00	45.15	B
4855	NE	ARG	B1151	26.864	20.392	-7.230	1.00	51.00	B
4856	CZ	ARG	B1151	27.015	21.210	-8.282	1.00	48.46	B
4857	NH1	ARG	B1151	26.647	22.516	-8.167	1.00	44.69	B
4858	NH2	ARG	B1151	27.683	20.770	-9.405	1.00	45.95	B
4859	C	ARG	B1151	23.696	21.210	-2.609	1.00	58.29	B

4860	O	ARG	B1151	23.350	22.285	-1.999	1.00	57.14	B
4861	N	TYR	B1152	24.303	20.091	-2.072	1.00	57.01	B
4862	CA	TYR	B1152	24.416	19.804	-0.624	1.00	56.46	B
4863	CB	TYR	B1152	24.122	18.276	-0.147	1.00	56.05	B
4864	CG	TYR	B1152	22.609	18.039	0.121	1.00	50.06	B
4865	CD1	TYR	B1152	21.775	17.572	-0.899	1.00	51.65	B
4866	CE1	TYR	B1152	20.364	17.434	-0.751	1.00	44.50	B
4867	CD2	TYR	B1152	22.043	18.375	1.305	1.00	38.75	B
4868	CE2	TYR	B1152	20.616	18.309	1.458	1.00	45.21	B
4869	CZ	TYR	B1152	19.782	17.830	0.378	1.00	45.80	B
4870	OH	TYR	B1152	18.401	17.673	0.513	1.00	39.69	B
4871	C	TYR	B1152	25.787	20.163	-0.193	1.00	58.08	B
4872	O	TYR	B1152	26.814	19.871	-0.895	1.00	57.18	B
4873	N	ALA	B1153	25.793	20.725	1.027	1.00	59.39	B
4874	CA	ALA	B1153	26.974	21.396	1.535	1.00	60.62	B
4875	CB	ALA	B1153	26.561	22.791	1.956	1.00	58.58	B
4876	C	ALA	B1153	27.664	20.693	2.696	1.00	61.34	B
4877	O	ALA	B1153	27.119	20.867	3.795	1.00	64.42	B
4878	N	HIS	B1154	28.864	20.053	2.506	1.00	62.19	B
4879	CA	HIS	B1154	29.574	19.087	3.475	1.00	62.48	B
4880	CB	HIS	B1154	29.869	17.726	2.849	1.00	63.02	B
4881	CG	HIS	B1154	30.807	17.746	1.674	1.00	61.92	B
4882	CD2	HIS	B1154	31.769	16.849	1.308	1.00	63.04	B
4883	ND1	HIS	B1154	30.694	18.644	0.599	1.00	58.83	B
4884	CE1	HIS	B1154	31.613	18.347	-0.325	1.00	52.73	B
4885	NE2	HIS	B1154	32.264	17.245	0.066	1.00	55.83	B
4886	C	HIS	B1154	30.940	19.426	3.786	1.00	63.46	B
4887	O	HIS	B1154	31.567	19.973	2.908	1.00	62.28	B
4888	N	LEU	B1155	31.468	18.960	4.950	1.00	64.83	B
4889	CA	LEU	B1155	32.705	19.609	5.585	1.00	62.12	B
4890	CB	LEU	B1155	32.861	19.397	7.141	1.00	62.68	B
4891	CG	LEU	B1155	33.233	20.566	8.263	1.00	63.40	B
4892	CD1	LEU	B1155	32.465	21.762	8.216	1.00	56.90	B
4893	CD2	LEU	B1155	33.334	20.297	9.847	1.00	57.70	B
4894	C	LEU	B1155	33.924	19.259	4.876	1.00	62.90	B
4895	O	LEU	B1155	34.765	18.683	5.488	1.00	65.20	B
4896	N	SER	B1156	34.047	19.626	3.610	1.00	63.14	B
4897	CA	SER	B1156	35.132	19.258	2.727	1.00	66.60	B
4898	CB	SER	B1156	35.624	20.527	2.140	1.00	68.01	B
4899	OG	SER	B1156	35.525	20.433	0.714	1.00	76.63	B
4900	C	SER	B1156	36.398	18.626	3.277	1.00	69.43	B
4901	O	SER	B1156	36.928	18.961	4.421	1.00	69.50	B
4902	N	ALA	B1157	36.987	17.791	2.435	1.00	70.75	B
4903	CA	ALA	B1157	38.205	17.099	2.876	1.00	72.13	B
4904	CB	ALA	B1157	38.414	15.941	1.983	1.00	73.34	B
4905	C	ALA	B1157	39.553	17.952	3.013	1.00	73.68	B
4906	O	ALA	B1157	39.615	19.056	3.677	1.00	72.33	B
4907	N	ARG	B1158	40.616	17.406	2.372	1.00	74.32	B
4908	CA	ARG	B1158	41.915	18.085	2.153	1.00	73.77	B
4909	CB	ARG	B1158	42.425	17.959	0.695	1.00	73.11	B
4910	CG	ARG	B1158	42.450	16.543	-0.014	1.00	73.51	B
4911	CD	ARG	B1158	43.490	15.501	0.619	1.00	72.93	B
4912	NE	ARG	B1158	42.833	14.222	0.890	1.00	75.12	B
4913	CZ	ARG	B1158	43.370	13.141	1.458	1.00	78.02	B
4914	NH1	ARG	B1158	44.650	13.148	1.877	1.00	77.66	B
4915	NH2	ARG	B1158	42.584	12.035	1.587	1.00	75.36	B

4916	C	ARG	B1158	41.768	19.545	2.497	1.00	74.10	B
4917	O	ARG	B1158	42.263	19.991	3.541	1.00	74.12	B
4918	N	PRO	B1159	41.053	20.304	1.627	1.00	75.39	B
4919	CD	PRO	B1159	40.492	19.970	0.285	1.00	75.32	B
4920	CA	PRO	B1159	40.648	21.676	2.059	1.00	75.22	B
4921	CB	PRO	B1159	39.453	21.966	1.109	1.00	75.69	B
4922	CG	PRO	B1159	39.182	20.619	0.292	1.00	72.50	B
4923	C	PRO	B1159	40.342	21.871	3.640	1.00	75.69	B
4924	O	PRO	B1159	39.285	21.397	4.180	1.00	74.86	B
4925	N	ALA	B1160	41.327	22.483	4.346	1.00	75.34	B
4926	CA	ALA	B1160	41.298	22.886	5.857	1.00	74.29	B
4927	CB	ALA	B1160	42.616	23.582	6.209	1.00	73.88	B
4928	C	ALA	B1160	40.180	23.782	6.478	1.00	72.51	B
4929	O	ALA	B1160	40.182	25.002	6.276	1.00	71.76	B
4930	N	ASP	B1161	39.273	23.246	7.277	1.00	72.31	B
4931	CA	ASP	B1161	38.122	24.097	7.648	1.00	71.81	B
4932	CB	ASP	B1161	38.682	25.462	8.144	1.00	73.28	B
4933	CG	ASP	B1161	37.592	26.495	8.303	1.00	76.86	B
4934	OD1	ASP	B1161	36.412	26.002	8.471	1.00	76.69	B
4935	OD2	ASP	B1161	37.898	27.748	8.171	1.00	78.61	B
4936	C	ASP	B1161	37.236	24.362	6.436	1.00	70.67	B
4937	O	ASP	B1161	37.826	24.534	5.345	1.00	72.10	B
4938	N	GLU	B1162	35.884	24.453	6.544	1.00	68.43	B
4939	CA	GLU	B1162	35.033	24.717	5.258	1.00	67.81	B
4940	CB	GLU	B1162	35.824	24.336	3.933	1.00	67.10	B
4941	CG	GLU	B1162	35.502	25.145	2.645	1.00	67.98	B
4942	CD	GLU	B1162	36.704	25.521	1.765	1.00	68.89	B
4943	OE1	GLU	B1162	37.474	24.560	1.321	1.00	64.08	B
4944	OE2	GLU	B1162	36.855	26.801	1.492	1.00	70.67	B
4945	C	GLU	B1162	33.561	24.197	5.052	1.00	65.90	B
4946	O	GLU	B1162	32.803	23.814	5.942	1.00	66.47	B
4947	N	ILE	B1163	33.120	24.177	3.821	1.00	64.15	B
4948	CA	ILE	B1163	31.744	23.877	3.616	1.00	62.73	B
4949	CB	ILE	B1163	30.784	24.722	4.470	1.00	62.40	B
4950	CG2	ILE	B1163	29.282	23.990	4.595	1.00	63.74	B
4951	CG1	ILE	B1163	31.322	24.904	5.846	1.00	58.15	B
4952	CD1	ILE	B1163	30.446	25.796	6.627	1.00	59.20	B
4953	C	ILE	B1163	31.285	23.734	2.132	1.00	62.12	B
4954	O	ILE	B1163	30.075	24.005	1.808	1.00	60.21	B
4955	N	ALA	B1164	32.203	23.163	1.319	1.00	60.36	B
4956	CA	ALA	B1164	31.903	22.788	-0.105	1.00	61.45	B
4957	CB	ALA	B1164	32.968	21.877	-0.615	1.00	63.49	B
4958	C	ALA	B1164	30.485	22.206	-0.418	1.00	60.79	B
4959	O	ALA	B1164	29.973	21.170	0.185	1.00	61.99	B
4960	N	VAL	B1165	29.813	22.922	-1.276	1.00	56.08	B
4961	CA	VAL	B1165	28.451	22.639	-1.425	1.00	54.86	B
4962	CB	VAL	B1165	27.596	23.917	-1.306	1.00	54.58	B
4963	CG1	VAL	B1165	26.021	23.577	-1.511	1.00	53.27	B
4964	CG2	VAL	B1165	27.824	24.546	-0.094	1.00	51.69	B
4965	C	VAL	B1165	28.279	21.981	-2.794	1.00	54.82	B
4966	O	VAL	B1165	27.506	22.480	-3.610	1.00	54.00	B
4967	N	ASP	B1166	28.991	20.843	-3.009	1.00	57.17	B
4968	CA	ASP	B1166	29.187	20.102	-4.338	1.00	57.21	B
4969	CB	ASP	B1166	30.647	20.182	-4.938	1.00	55.19	B
4970	CG	ASP	B1166	31.739	19.435	-4.023	1.00	64.88	B
4971	OD1	ASP	B1166	31.488	19.202	-2.788	1.00	74.98	B

4972	OD2	ASP	B1166	32.892	19.140	-4.452	1.00	65.35	B
4973	C	ASP	B1166	28.740	18.652	-4.232	1.00	57.23	B
4974	O	ASP	B1166	29.475	17.701	-4.568	1.00	59.84	B
4975	N	ARG	B1167	27.560	18.398	-3.758	1.00	57.11	B
4976	CA	ARG	B1167	27.305	16.949	-3.643	1.00	56.20	B
4977	CB	ARG	B1167	28.062	16.398	-2.378	1.00	56.90	B
4978	CG	ARG	B1167	27.619	16.966	-1.048	1.00	55.74	B
4979	CD	ARG	B1167	27.198	15.777	-0.203	1.00	63.75	B
4980	NE	ARG	B1167	28.328	14.923	0.272	1.00	68.30	B
4981	CZ	ARG	B1167	28.517	14.455	1.535	1.00	65.43	B
4982	NH1	ARG	B1167	27.622	14.694	2.501	1.00	59.52	B
4983	NH2	ARG	B1167	29.634	13.748	1.827	1.00	65.11	B
4984	C	ARG	B1167	25.808	16.688	-3.662	1.00	56.12	B
4985	O	ARG	B1167	25.003	17.467	-3.118	1.00	56.47	B
4986	N	ASP	B1168	25.381	15.649	-4.353	1.00	57.27	B
4987	CA	ASP	B1168	23.945	15.553	-4.561	1.00	58.14	B
4988	CB	ASP	B1168	23.366	14.498	-5.608	1.00	57.24	B
4989	CG	ASP	B1168	24.030	13.037	-5.591	1.00	57.06	B
4990	OD1	ASP	B1168	25.294	12.940	-5.400	1.00	54.25	B
4991	OD2	ASP	B1168	23.274	11.996	-5.928	1.00	47.05	B
4992	C	ASP	B1168	23.317	15.349	-3.246	1.00	58.18	B
4993	O	ASP	B1168	22.155	15.653	-3.094	1.00	59.93	B
4994	N	VAL	B1169	24.016	14.686	-2.353	1.00	56.75	B
4995	CA	VAL	B1169	23.279	14.171	-1.231	1.00	56.52	B
4996	CB	VAL	B1169	22.566	12.822	-1.494	1.00	54.41	B
4997	CG1	VAL	B1169	23.514	11.644	-1.728	1.00	56.66	B
4998	CG2	VAL	B1169	21.772	12.588	-0.360	1.00	58.02	B
4999	C	VAL	B1169	24.153	14.243	-0.082	1.00	54.47	B
5000	O	VAL	B1169	25.391	14.271	-0.320	1.00	57.01	B
5001	N	PRO	B1170	23.570	14.394	1.127	1.00	52.30	B
5002	CD	PRO	B1170	22.124	14.347	1.461	1.00	50.51	B
5003	CA	PRO	B1170	24.384	14.657	2.325	1.00	49.97	B
5004	CB	PRO	B1170	23.358	15.364	3.315	1.00	49.10	B
5005	CG	PRO	B1170	22.078	14.732	3.009	1.00	44.98	B
5006	C	PRO	B1170	24.573	13.250	2.808	1.00	49.59	B
5007	O	PRO	B1170	23.820	12.780	3.543	1.00	49.70	B
5008	N	TRP	B1171	25.577	12.545	2.399	1.00	50.44	B
5009	CA	TRP	B1171	25.784	11.272	2.977	1.00	49.04	B
5010	CB	TRP	B1171	26.039	10.360	1.735	1.00	48.41	B
5011	CG	TRP	B1171	25.307	9.080	1.849	1.00	45.07	B
5012	CD2	TRP	B1171	23.878	8.967	1.801	1.00	37.88	B
5013	CE2	TRP	B1171	23.561	7.566	1.961	1.00	41.15	B
5014	CE3	TRP	B1171	22.842	9.912	1.583	1.00	34.77	B
5015	CD1	TRP	B1171	25.839	7.768	2.041	1.00	38.99	B
5016	NE1	TRP	B1171	24.768	6.883	2.133	1.00	48.14	B
5017	CZ2	TRP	B1171	22.252	7.076	1.900	1.00	36.51	B
5018	CZ3	TRP	B1171	21.495	9.484	1.618	1.00	36.51	B
5019	CH2	TRP	B1171	21.212	8.018	1.792	1.00	42.35	B
5020	C	TRP	B1171	27.019	11.220	3.898	1.00	47.87	B
5021	O	TRP	B1171	27.987	10.828	3.403	1.00	48.58	B
5022	N	GLY	B1172	26.973	11.560	5.195	1.00	47.59	B
5023	CA	GLY	B1172	27.993	11.137	6.178	1.00	45.94	B
5024	C	GLY	B1172	28.141	12.049	7.409	1.00	47.54	B
5025	O	GLY	B1172	27.163	12.841	7.764	1.00	46.74	B
5026	N	VAL	B1173	29.314	11.964	8.102	1.00	44.61	B
5027	CA	VAL	B1173	29.573	12.941	9.077	1.00	46.16	B

5028	CB	VAL	B1173	30.843	12.713	10.062	1.00	47.94	B
5029	CG1	VAL	B1173	30.426	12.751	11.604	1.00	46.53	B
5030	CG2	VAL	B1173	32.008	11.693	9.644	1.00	47.64	B
5031	C	VAL	B1173	29.603	14.427	8.482	1.00	49.13	B
5032	O	VAL	B1173	29.069	15.405	9.116	1.00	47.22	B
5033	N	ASP	B1174	30.334	14.652	7.373	1.00	50.05	B
5034	CA	ASP	B1174	30.081	15.881	6.635	1.00	51.49	B
5035	CB	ASP	B1174	30.439	15.645	5.228	1.00	49.80	B
5036	CG	ASP	B1174	31.428	14.617	5.136	1.00	51.90	B
5037	OD1	ASP	B1174	32.532	14.859	5.729	1.00	48.53	B
5038	OD2	ASP	B1174	31.097	13.589	4.469	1.00	50.54	B
5039	C	ASP	B1174	28.630	16.428	6.539	1.00	52.61	B
5040	O	ASP	B1174	28.349	17.167	5.579	1.00	51.92	B
5041	N	SER	B1175	27.700	16.179	7.443	1.00	51.51	B
5042	CA	SER	B1175	26.586	17.000	7.159	1.00	51.56	B
5043	CB	SER	B1175	25.575	16.265	6.242	1.00	53.00	B
5044	OG	SER	B1175	26.336	15.790	5.013	1.00	51.34	B
5045	C	SER	B1175	26.126	17.548	8.427	1.00	52.58	B
5046	O	SER	B1175	25.706	18.767	8.616	1.00	51.67	B
5047	N	LEU	B1176	26.242	16.672	9.400	1.00	54.73	B
5048	CA	LEU	B1176	25.668	17.089	10.724	1.00	54.53	B
5049	CB	LEU	B1176	25.780	16.037	11.721	1.00	52.36	B
5050	CG	LEU	B1176	25.066	16.421	12.958	1.00	52.29	B
5051	CD1	LEU	B1176	23.599	16.763	12.729	1.00	53.20	B
5052	CD2	LEU	B1176	25.207	15.380	14.016	1.00	55.15	B
5053	C	LEU	B1176	26.315	18.438	11.098	1.00	56.89	B
5054	O	LEU	B1176	27.571	18.529	10.910	1.00	55.00	B
5055	N	ILE	B1177	25.447	19.482	11.342	1.00	58.02	B
5056	CA	ILE	B1177	25.852	20.735	11.838	1.00	60.78	B
5057	CB	ILE	B1177	25.486	21.882	10.945	1.00	62.68	B
5058	CG2	ILE	B1177	24.964	23.262	11.816	1.00	60.44	B
5059	CG1	ILE	B1177	26.683	22.246	10.106	1.00	64.46	B
5060	CD1	ILE	B1177	27.887	22.598	10.951	1.00	60.83	B
5061	C	ILE	B1177	25.032	21.071	12.989	1.00	64.17	B
5062	O	ILE	B1177	23.747	20.894	12.930	1.00	61.74	B
5063	N	THR	B1178	25.739	21.695	13.973	1.00	65.74	B
5064	CA	THR	B1178	25.044	22.042	15.248	1.00	68.16	B
5065	CB	THR	B1178	25.580	21.160	16.445	1.00	69.28	B
5066	OG1	THR	B1178	26.195	19.907	15.948	1.00	73.30	B
5067	CG2	THR	B1178	24.393	20.807	17.435	1.00	67.53	B
5068	C	THR	B1178	24.795	23.554	15.579	1.00	67.67	B
5069	O	THR	B1178	25.609	24.344	15.355	1.00	69.24	B
5070	N	LEU	B1179	23.627	23.938	16.069	1.00	67.37	B
5071	CA	LEU	B1179	23.142	25.342	16.210	1.00	66.19	B
5072	CB	LEU	B1179	21.778	25.641	15.432	1.00	64.43	B
5073	CG	LEU	B1179	21.685	25.636	13.901	1.00	63.78	B
5074	CD1	LEU	B1179	20.419	26.249	13.492	1.00	68.71	B
5075	CD2	LEU	B1179	22.855	26.371	13.160	1.00	59.53	B
5076	C	LEU	B1179	22.771	25.434	17.651	1.00	65.69	B
5077	O	LEU	B1179	21.593	25.263	17.971	1.00	61.26	B
5078	N	ALA	B1180	23.730	25.651	18.553	1.00	66.92	B
5079	CA	ALA	B1180	23.229	25.543	19.929	1.00	68.83	B
5080	CB	ALA	B1180	23.857	24.310	20.728	1.00	68.51	B
5081	C	ALA	B1180	23.351	26.934	20.578	1.00	68.71	B
5082	O	ALA	B1180	23.806	27.865	19.855	1.00	69.04	B
5083	N	PHE	B1181	22.882	27.125	21.828	1.00	67.23	B

5084	CA	PHE	B1181	22.747	28.493	22.325	1.00	66.78	B
5085	CB	PHE	B1181	22.190	28.479	23.676	1.00	65.44	B
5086	CG	PHE	B1181	20.822	27.829	23.707	1.00	67.32	B
5087	CD1	PHE	B1181	19.915	28.056	22.682	1.00	63.04	B
5088	CD2	PHE	B1181	20.445	27.026	24.720	1.00	64.17	B
5089	CE1	PHE	B1181	18.694	27.546	22.695	1.00	60.93	B
5090	CE2	PHE	B1181	19.232	26.554	24.721	1.00	68.19	B
5091	CZ	PHE	B1181	18.319	26.822	23.702	1.00	64.91	B
5092	C	PHE	B1181	24.062	29.189	22.279	1.00	68.44	B
5093	O	PHE	B1181	25.135	28.561	22.538	1.00	68.27	B
5094	N	GLN	B1182	24.060	30.437	21.797	1.00	68.03	B
5095	CA	GLN	B1182	25.204	31.235	22.179	1.00	66.43	B
5096	CB	GLN	B1182	25.714	32.012	20.978	1.00	64.98	B
5097	CG	GLN	B1182	26.814	31.261	20.321	1.00	69.22	B
5098	CD	GLN	B1182	28.119	32.105	20.015	1.00	73.97	B
5099	OE1	GLN	B1182	28.229	33.292	20.382	1.00	77.27	B
5100	NE2	GLN	B1182	29.102	31.474	19.355	1.00	67.36	B
5101	C	GLN	B1182	24.987	32.120	23.470	1.00	66.45	B
5102	O	GLN	B1182	24.486	31.736	24.612	1.00	63.70	B
5103	N	ASP	B1183	25.370	33.356	23.256	1.00	67.03	B
5104	CA	ASP	B1183	25.647	34.194	24.368	1.00	69.64	B
5105	CB	ASP	B1183	26.887	35.099	24.110	1.00	67.88	B
5106	CG	ASP	B1183	27.311	35.116	22.591	1.00	66.51	B
5107	OD1	ASP	B1183	26.406	35.162	21.604	1.00	51.11	B
5108	OD2	ASP	B1183	28.562	35.023	22.476	1.00	56.49	B
5109	C	ASP	B1183	24.351	34.911	24.419	1.00	71.57	B
5110	O	ASP	B1183	24.303	36.095	24.640	1.00	72.77	B
5111	N	GLN	B1184	23.283	34.153	24.175	1.00	73.81	B
5112	CA	GLN	B1184	22.116	34.757	23.463	1.00	74.78	B
5113	CB	GLN	B1184	21.832	36.179	24.033	1.00	72.28	B
5114	CG	GLN	B1184	21.273	36.181	25.546	1.00	72.20	B
5115	CD	GLN	B1184	19.730	35.650	25.748	1.00	76.24	B
5116	OE1	GLN	B1184	18.778	36.465	26.072	1.00	69.72	B
5117	NE2	GLN	B1184	19.520	34.274	25.582	1.00	74.79	B
5118	C	GLN	B1184	22.010	34.714	21.866	1.00	73.84	B
5119	O	GLN	B1184	20.977	35.015	21.394	1.00	75.38	B
5120	N	ARG	B1185	23.038	34.410	21.070	1.00	73.99	B
5121	CA	ARG	B1185	22.920	34.562	19.557	1.00	75.06	B
5122	CB	ARG	B1185	24.200	34.994	18.854	1.00	74.71	B
5123	CG	ARG	B1185	24.497	36.461	18.786	1.00	73.16	B
5124	CD	ARG	B1185	25.195	36.534	17.453	1.00	77.00	B
5125	NE	ARG	B1185	24.999	37.821	16.696	1.00	87.06	B
5126	CZ	ARG	B1185	24.173	38.124	15.661	1.00	82.00	B
5127	NH1	ARG	B1185	23.331	37.286	15.089	1.00	77.45	B
5128	NH2	ARG	B1185	24.202	39.352	15.184	1.00	85.40	B
5129	C	ARG	B1185	22.484	33.267	18.856	1.00	75.69	B
5130	O	ARG	B1185	21.276	32.986	18.768	1.00	77.37	B
5131	N	TYR	B1186	23.453	32.496	18.345	1.00	74.20	B
5132	CA	TYR	B1186	23.200	31.080	17.965	1.00	72.40	B
5133	CB	TYR	B1186	21.781	30.973	17.342	1.00	71.03	B
5134	CG	TYR	B1186	20.742	30.468	18.233	1.00	62.98	B
5135	CD1	TYR	B1186	20.723	29.151	18.606	1.00	58.13	B
5136	CE1	TYR	B1186	19.752	28.705	19.514	1.00	63.92	B
5137	CD2	TYR	B1186	19.815	31.330	18.738	1.00	55.24	B
5138	CE2	TYR	B1186	18.873	30.944	19.612	1.00	55.26	B
5139	CZ	TYR	B1186	18.781	29.608	20.001	1.00	62.64	B

5140	OH	TYR	B1186	17.743	29.181	20.847	1.00	60.02	B
5141	C	TYR	B1186	24.220	30.448	16.940	1.00	72.33	B
5142	O	TYR	B1186	23.898	30.257	15.731	1.00	72.81	B
5143	N	SER	B1187	25.419	30.130	17.418	1.00	71.14	B
5144	CA	SER	B1187	26.456	29.566	16.562	1.00	70.26	B
5145	CB	SER	B1187	27.665	29.349	17.403	1.00	70.80	B
5146	OG	SER	B1187	27.758	28.054	17.913	1.00	65.93	B
5147	C	SER	B1187	26.164	28.245	15.743	1.00	70.53	B
5148	O	SER	B1187	24.990	27.717	15.665	1.00	70.23	B
5149	N	VAL	B1188	27.271	27.724	15.155	1.00	67.55	B
5150	CA	VAL	B1188	27.182	26.682	14.138	1.00	61.21	B
5151	CB	VAL	B1188	27.024	27.243	12.778	1.00	57.23	B
5152	CG1	VAL	B1188	25.974	28.149	12.908	1.00	53.10	B
5153	CG2	VAL	B1188	28.264	27.922	12.402	1.00	54.13	B
5154	C	VAL	B1188	28.353	25.777	14.207	1.00	61.91	B
5155	O	VAL	B1188	29.285	25.896	13.405	1.00	64.50	B
5156	N	GLN	B1189	28.263	24.832	15.108	1.00	61.15	B
5157	CA	GLN	B1189	29.342	23.879	15.420	1.00	63.51	B
5158	CB	GLN	B1189	29.061	23.257	16.808	1.00	62.02	B
5159	CG	GLN	B1189	29.730	21.959	17.021	1.00	60.53	B
5160	CD	GLN	B1189	29.211	21.275	18.274	1.00	68.31	B
5161	OE1	GLN	B1189	29.166	21.883	19.396	1.00	70.12	B
5162	NE2	GLN	B1189	28.786	19.990	18.108	1.00	67.19	B
5163	C	GLN	B1189	29.601	22.807	14.308	1.00	64.43	B
5164	O	GLN	B1189	28.825	21.856	14.137	1.00	67.10	B
5165	N	THR	B1190	30.631	22.962	13.527	1.00	65.33	B
5166	CA	THR	B1190	31.029	21.926	12.544	1.00	69.17	B
5167	CB	THR	B1190	32.519	22.158	12.284	1.00	70.80	B
5168	OG1	THR	B1190	33.152	22.571	13.536	1.00	76.36	B
5169	CG2	THR	B1190	32.711	23.221	11.276	1.00	69.09	B
5170	C	THR	B1190	31.011	20.406	12.980	1.00	69.88	B
5171	O	THR	B1190	30.013	19.899	13.570	1.00	70.24	B
5172	N	ALA	B1191	32.123	19.654	12.762	1.00	67.79	B
5173	CA	ALA	B1191	31.954	18.197	13.001	1.00	67.16	B
5174	CB	ALA	B1191	32.746	17.373	11.919	1.00	66.67	B
5175	C	ALA	B1191	32.276	17.642	14.434	1.00	65.02	B
5176	O	ALA	B1191	31.916	16.529	14.789	1.00	62.69	B
5177	N	ASP	B1192	32.889	18.487	15.231	1.00	63.61	B
5178	CA	ASP	B1192	34.085	18.149	15.934	1.00	61.13	B
5179	CB	ASP	B1192	35.262	18.147	14.908	1.00	61.71	B
5180	CG	ASP	B1192	35.511	19.592	14.135	1.00	56.03	B
5181	OD1	ASP	B1192	34.859	20.617	14.397	1.00	55.47	B
5182	OD2	ASP	B1192	36.425	19.691	13.269	1.00	43.37	B
5183	C	ASP	B1192	34.193	19.370	16.753	1.00	60.78	B
5184	O	ASP	B1192	35.278	19.855	16.961	1.00	61.28	B
5185	N	HIS	B1193	33.045	19.972	17.004	1.00	60.11	B
5186	CA	HIS	B1193	32.835	20.934	18.084	1.00	60.11	B
5187	CB	HIS	B1193	33.566	20.455	19.304	1.00	58.79	B
5188	CG	HIS	B1193	32.957	19.210	19.900	1.00	60.16	B
5189	CD2	HIS	B1193	31.790	19.027	20.602	1.00	58.77	B
5190	ND1	HIS	B1193	33.521	17.949	19.765	1.00	57.05	B
5191	CE1	HIS	B1193	32.737	17.048	20.375	1.00	57.17	B
5192	NE2	HIS	B1193	31.686	17.669	20.894	1.00	52.86	B
5193	C	HIS	B1193	33.042	22.430	17.746	1.00	60.17	B
5194	O	HIS	B1193	32.319	23.305	18.234	1.00	59.66	B
5195	N	ARG	B1194	33.951	22.685	16.818	1.00	60.63	B

5196	CA	ARG	B1194	34.419	24.057	16.554	1.00	61.63	B
5197	CB	ARG	B1194	35.920	24.120	15.983	1.00	60.52	B
5198	CG	ARG	B1194	36.268	22.945	15.086	1.00	57.21	B
5199	CD	ARG	B1194	37.659	23.135	14.237	1.00	64.97	B
5200	NE	ARG	B1194	37.564	22.700	12.753	1.00	64.47	B
5201	CZ	ARG	B1194	38.326	23.098	11.717	1.00	53.20	B
5202	NH1	ARG	B1194	39.339	23.952	11.822	1.00	51.70	B
5203	NH2	ARG	B1194	38.052	22.624	10.548	1.00	50.09	B
5204	C	ARG	B1194	33.341	24.830	15.721	1.00	61.10	B
5205	O	ARG	B1194	32.554	24.210	14.949	1.00	62.40	B
5206	N	PHE	B1195	33.399	26.143	15.836	1.00	59.05	B
5207	CA	PHE	B1195	32.315	26.955	15.629	1.00	58.39	B
5208	CB	PHE	B1195	32.200	27.675	16.882	1.00	58.85	B
5209	CG	PHE	B1195	32.126	26.789	18.152	1.00	61.76	B
5210	CD1	PHE	B1195	33.260	26.541	18.927	1.00	62.70	B
5211	CD2	PHE	B1195	30.870	26.398	18.701	1.00	64.66	B
5212	CE1	PHE	B1195	33.161	25.822	20.191	1.00	65.05	B
5213	CE2	PHE	B1195	30.774	25.658	19.936	1.00	65.10	B
5214	CZ	PHE	B1195	31.912	25.373	20.681	1.00	61.99	B
5215	C	PHE	B1195	32.679	27.940	14.579	1.00	59.02	B
5216	O	PHE	B1195	33.800	28.463	14.576	1.00	59.18	B
5217	N	LEU	B1196	31.783	28.207	13.620	1.00	61.21	B
5218	CA	LEU	B1196	31.964	29.399	12.647	1.00	60.50	B
5219	CB	LEU	B1196	30.808	29.452	11.648	1.00	60.63	B
5220	CG	LEU	B1196	31.322	29.810	10.234	1.00	60.41	B
5221	CD1	LEU	B1196	32.314	28.644	9.857	1.00	54.21	B
5222	CD2	LEU	B1196	29.952	29.697	9.526	1.00	60.92	B
5223	C	LEU	B1196	32.025	30.853	13.202	1.00	59.80	B
5224	O	LEU	B1196	31.139	31.280	13.914	1.00	59.04	B
5225	N	ARG	B1197	33.034	31.627	12.835	1.00	61.17	B
5226	CA	ARG	B1197	32.981	33.068	13.065	1.00	61.23	B
5227	CB	ARG	B1197	34.395	33.639	13.452	1.00	63.28	B
5228	CG	ARG	B1197	34.560	35.289	13.297	1.00	62.64	B
5229	CD	ARG	B1197	36.025	35.736	13.057	1.00	63.62	B
5230	NE	ARG	B1197	36.944	34.932	13.855	1.00	67.96	B
5231	CZ	ARG	B1197	37.937	34.225	13.334	1.00	62.03	B
5232	NH1	ARG	B1197	38.137	34.335	12.050	1.00	59.59	B
5233	NH2	ARG	B1197	38.743	33.493	14.107	1.00	54.12	B
5234	C	ARG	B1197	32.733	33.505	11.708	1.00	60.28	B
5235	O	ARG	B1197	33.278	32.895	10.758	1.00	59.90	B
5236	N	HIS	B1198	32.020	34.590	11.592	1.00	62.22	B
5237	CA	HIS	B1198	31.636	35.137	10.241	1.00	66.67	B
5238	CB	HIS	B1198	30.783	36.382	10.391	1.00	64.94	B
5239	CG	HIS	B1198	31.271	37.322	11.462	1.00	72.94	B
5240	CD2	HIS	B1198	32.147	38.363	11.400	1.00	77.15	B
5241	ND1	HIS	B1198	30.802	37.305	12.767	1.00	74.29	B
5242	CE1	HIS	B1198	31.354	38.304	13.443	1.00	76.99	B
5243	NE2	HIS	B1198	32.128	38.993	12.622	1.00	76.12	B
5244	C	HIS	B1198	32.773	35.402	9.262	1.00	68.24	B
5245	O	HIS	B1198	32.954	36.571	8.723	1.00	71.98	B
5246	N	ASP	B1199	33.600	34.371	9.043	1.00	69.42	B
5247	CA	ASP	B1199	34.863	34.603	8.313	1.00	67.97	B
5248	CB	ASP	B1199	35.985	35.185	9.228	1.00	66.27	B
5249	CG	ASP	B1199	37.137	34.234	9.413	1.00	64.18	B
5250	OD1	ASP	B1199	38.347	34.621	9.509	1.00	50.97	B
5251	OD2	ASP	B1199	36.769	33.047	9.464	1.00	66.34	B

5252	C	ASP	B1199	35.357	33.457	7.348	1.00	68.77	B
5253	O	ASP	B1199	36.512	33.648	6.745	1.00	65.84	B
5254	N	GLY	B1200	34.490	32.393	7.146	1.00	67.85	B
5255	CA	GLY	B1200	34.896	31.013	6.557	1.00	68.84	B
5256	C	GLY	B1200	35.743	29.925	7.357	1.00	68.75	B
5257	O	GLY	B1200	36.379	28.944	6.843	1.00	66.66	B
5258	N	ARG	B1201	35.713	30.105	8.662	1.00	68.93	B
5259	CA	ARG	B1201	36.717	29.518	9.492	1.00	67.55	B
5260	CB	ARG	B1201	37.803	30.590	9.860	1.00	69.26	B
5261	CG	ARG	B1201	39.069	30.728	8.756	1.00	71.25	B
5262	CD	ARG	B1201	40.565	30.335	9.403	1.00	67.30	B
5263	NE	ARG	B1201	40.389	30.153	10.817	1.00	67.36	B
5264	CZ	ARG	B1201	39.743	29.118	11.384	1.00	68.68	B
5265	NH1	ARG	B1201	39.577	29.109	12.727	1.00	65.40	B
5266	NH2	ARG	B1201	39.273	28.087	10.616	1.00	62.72	B
5267	C	ARG	B1201	36.137	28.749	10.692	1.00	65.68	B
5268	O	ARG	B1201	34.895	28.803	11.061	1.00	64.37	B
5269	N	LEU	B1202	37.043	27.931	11.238	1.00	64.35	B
5270	CA	LEU	B1202	36.704	27.095	12.408	1.00	60.92	B
5271	CB	LEU	B1202	36.383	25.666	11.921	1.00	59.77	B
5272	CG	LEU	B1202	34.973	24.990	11.804	1.00	55.47	B
5273	CD1	LEU	B1202	35.191	23.537	12.544	1.00	45.59	B
5274	CD2	LEU	B1202	33.722	25.784	12.398	1.00	43.52	B
5275	C	LEU	B1202	37.736	27.296	13.559	1.00	59.15	B
5276	O	LEU	B1202	38.915	27.075	13.467	1.00	54.93	B
5277	N	VAL	B1203	37.273	27.928	14.607	1.00	62.39	B
5278	CA	VAL	B1203	38.195	28.294	15.797	1.00	63.20	B
5279	CB	VAL	B1203	37.666	29.381	16.732	1.00	61.66	B
5280	CG1	VAL	B1203	37.295	30.674	15.982	1.00	63.82	B
5281	CG2	VAL	B1203	36.461	28.898	17.501	1.00	58.28	B
5282	C	VAL	B1203	38.263	27.087	16.708	1.00	65.37	B
5283	O	VAL	B1203	38.916	26.037	16.313	1.00	67.18	B
5284	N	ALA	B1204	37.549	27.213	17.860	1.00	64.73	B
5285	CA	ALA	B1204	37.881	26.462	19.116	1.00	65.60	B
5286	CB	ALA	B1204	38.845	27.224	19.942	1.00	66.68	B
5287	C	ALA	B1204	36.720	26.256	19.980	1.00	66.21	B
5288	O	ALA	B1204	36.084	25.134	19.941	1.00	65.59	B
5289	N	ARG	B1205	36.513	27.328	20.790	1.00	66.04	B
5290	CA	ARG	B1205	35.477	27.515	21.879	1.00	65.19	B
5291	CB	ARG	B1205	36.154	27.529	23.305	1.00	62.46	B
5292	CG	ARG	B1205	37.417	28.294	23.253	1.00	62.21	B
5293	CD	ARG	B1205	38.714	27.828	24.121	1.00	64.19	B
5294	NE	ARG	B1205	39.919	28.227	23.373	1.00	60.95	B
5295	CZ	ARG	B1205	40.017	29.347	22.626	1.00	69.25	B
5296	NH1	ARG	B1205	39.052	30.260	22.644	1.00	69.28	B
5297	NH2	ARG	B1205	41.124	29.634	21.903	1.00	75.42	B
5298	C	ARG	B1205	34.795	28.877	21.456	1.00	65.35	B
5299	O	ARG	B1205	35.433	29.742	20.825	1.00	65.26	B
5300	N	PRO	B1206	33.528	29.121	21.808	1.00	66.34	B
5301	CD	PRO	B1206	32.735	28.796	23.034	1.00	66.50	B
5302	CA	PRO	B1206	32.866	30.150	20.872	1.00	65.88	B
5303	CB	PRO	B1206	31.412	30.228	21.355	1.00	66.02	B
5304	CG	PRO	B1206	31.243	29.396	22.707	1.00	64.96	B
5305	C	PRO	B1206	33.532	31.532	21.101	1.00	66.60	B
5306	O	PRO	B1206	34.734	31.559	21.387	1.00	67.12	B
5307	N	GLU	B1207	32.797	32.636	21.032	1.00	65.27	B

5308	CA	GLU	B1207	33.385	33.973	21.215	1.00	65.25	B
5309	CB	GLU	B1207	34.761	34.147	20.489	1.00	63.95	B
5310	CG	GLU	B1207	34.821	34.291	18.997	1.00	60.46	B
5311	CD	GLU	B1207	35.684	33.200	18.506	1.00	56.03	B
5312	OE1	GLU	B1207	35.146	32.193	17.922	1.00	61.81	B
5313	OE2	GLU	B1207	36.881	33.227	18.885	1.00	52.58	B
5314	C	GLU	B1207	32.396	35.239	21.051	1.00	65.05	B
5315	O	GLU	B1207	31.175	35.105	21.286	1.00	66.30	B
5316	N	PRO	B1208	32.894	36.447	20.692	1.00	63.15	B
5317	CD	PRO	B1208	34.010	37.365	20.385	1.00	61.99	B
5318	CA	PRO	B1208	31.653	37.069	20.459	1.00	63.47	B
5319	CB	PRO	B1208	31.903	38.501	20.991	1.00	64.55	B
5320	CG	PRO	B1208	33.618	38.591	21.128	1.00	61.21	B
5321	C	PRO	B1208	31.459	36.943	18.893	1.00	64.00	B
5322	O	PRO	B1208	30.336	36.637	18.507	1.00	61.98	B
5323	N	ALA	B1209	32.566	37.088	18.088	1.00	64.00	B
5324	CA	ALA	B1209	32.688	37.361	16.512	1.00	63.00	B
5325	CB	ALA	B1209	33.925	38.177	16.196	1.00	60.78	B
5326	C	ALA	B1209	32.700	36.062	15.653	1.00	62.87	B
5327	O	ALA	B1209	33.651	35.782	14.953	1.00	60.14	B
5328	N	THR	B1210	31.562	35.317	15.843	1.00	65.38	B
5329	CA	THR	B1210	31.173	33.870	15.578	1.00	64.61	B
5330	CB	THR	B1210	31.863	33.077	16.589	1.00	64.74	B
5331	OG1	THR	B1210	33.217	33.182	16.227	1.00	70.21	B
5332	CG2	THR	B1210	31.314	31.599	16.737	1.00	61.68	B
5333	C	THR	B1210	29.630	33.409	15.599	1.00	64.46	B
5334	O	THR	B1210	29.314	32.414	14.974	1.00	67.46	B
5335	N	GLY	B1211	28.693	34.096	16.270	1.00	62.42	B
5336	CA	GLY	B1211	27.254	33.615	16.401	1.00	62.02	B
5337	C	GLY	B1211	25.974	34.315	15.819	1.00	60.76	B
5338	O	GLY	B1211	25.977	35.531	15.574	1.00	60.18	B
5339	N	TYR	B1212	24.853	33.590	15.668	1.00	60.27	B
5340	CA	TYR	B1212	23.810	34.149	14.788	1.00	62.56	B
5341	CB	TYR	B1212	23.792	33.524	13.426	1.00	60.37	B
5342	CG	TYR	B1212	25.202	33.262	12.999	1.00	59.89	B
5343	CD1	TYR	B1212	25.955	34.299	12.395	1.00	53.50	B
5344	CE1	TYR	B1212	27.350	34.099	12.088	1.00	65.28	B
5345	CD2	TYR	B1212	25.816	31.959	13.237	1.00	58.01	B
5346	CE2	TYR	B1212	27.153	31.703	12.863	1.00	58.90	B
5347	CZ	TYR	B1212	27.953	32.760	12.312	1.00	62.92	B
5348	OH	TYR	B1212	29.274	32.486	11.928	1.00	53.54	B
5349	C	TYR	B1212	22.396	34.257	15.272	1.00	64.57	B
5350	O	TYR	B1212	21.945	33.515	16.177	1.00	65.12	B
5351	N	THR	B1213	21.733	35.248	14.683	1.00	65.66	B
5352	CA	THR	B1213	20.365	35.552	14.997	1.00	67.41	B
5353	CB	THR	B1213	20.097	37.043	15.338	1.00	67.35	B
5354	OG1	THR	B1213	20.906	37.922	14.506	1.00	67.08	B
5355	CG2	THR	B1213	20.405	37.333	16.912	1.00	69.45	B
5356	C	THR	B1213	19.808	34.992	13.694	1.00	68.44	B
5357	O	THR	B1213	20.479	35.106	12.643	1.00	70.13	B
5358	N	LEU	B1214	18.736	34.197	13.801	1.00	68.80	B
5359	CA	LEU	B1214	18.170	33.498	12.666	1.00	66.92	B
5360	CB	LEU	B1214	17.785	32.075	13.083	1.00	65.18	B
5361	CG	LEU	B1214	18.769	31.137	13.852	1.00	56.00	B
5362	CD1	LEU	B1214	18.138	29.763	14.036	1.00	44.91	B
5363	CD2	LEU	B1214	20.041	31.003	13.175	1.00	48.70	B

5364	C	LEU	B1214	16.941	34.350	12.252	1.00	68.44	B
5365	O	LEU	B1214	15.877	34.270	12.949	1.00	69.13	B
5366	N	GLU	B1215	17.139	35.250	11.252	1.00	67.69	B
5367	CA	GLU	B1215	16.035	35.816	10.425	1.00	67.68	B
5368	CB	GLU	B1215	16.500	36.956	9.513	1.00	69.06	B
5369	CG	GLU	B1215	15.380	37.514	8.489	1.00	65.47	B
5370	CD	GLU	B1215	16.002	38.296	7.246	1.00	60.75	B
5371	OE1	GLU	B1215	15.206	38.764	6.439	1.00	48.55	B
5372	OE2	GLU	B1215	17.260	38.542	7.080	1.00	49.32	B
5373	C	GLU	B1215	15.460	34.681	9.535	1.00	70.70	B
5374	O	GLU	B1215	15.775	34.608	8.283	1.00	71.16	B
5375	N	PHE	B1216	14.684	33.783	10.181	1.00	69.96	B
5376	CA	PHE	B1216	14.045	32.720	9.497	1.00	68.74	B
5377	CB	PHE	B1216	13.150	31.935	10.476	1.00	68.69	B
5378	CG	PHE	B1216	13.890	30.858	11.279	1.00	71.28	B
5379	CD1	PHE	B1216	14.429	29.743	10.683	1.00	71.44	B
5380	CD2	PHE	B1216	14.045	30.955	12.664	1.00	75.22	B
5381	CE1	PHE	B1216	15.150	28.780	11.486	1.00	74.37	B
5382	CE2	PHE	B1216	14.763	29.948	13.458	1.00	70.89	B
5383	CZ	PHE	B1216	15.280	28.919	12.907	1.00	66.63	B
5384	C	PHE	B1216	13.243	33.509	8.426	1.00	70.15	B
5385	O	PHE	B1216	13.045	34.730	8.549	1.00	69.62	B
5386	N	ARG	B1217	12.767	32.835	7.377	1.00	70.27	B
5387	CA	ARG	B1217	12.174	33.503	6.321	1.00	68.74	B
5388	CB	ARG	B1217	13.311	33.931	5.376	1.00	68.58	B
5389	CG	ARG	B1217	13.515	35.399	5.424	1.00	67.67	B
5390	CD	ARG	B1217	12.283	36.121	4.810	1.00	71.88	B
5391	NE	ARG	B1217	11.127	36.351	5.708	1.00	76.95	B
5392	CZ	ARG	B1217	10.074	37.175	5.513	1.00	75.51	B
5393	NH1	ARG	B1217	9.937	37.925	4.414	1.00	74.37	B
5394	NH2	ARG	B1217	9.139	37.256	6.453	1.00	69.46	B
5395	C	ARG	B1217	11.218	32.546	5.679	1.00	69.39	B
5396	O	ARG	B1217	11.657	31.464	5.399	1.00	68.93	B
5397	N	SER	B1218	9.963	32.955	5.366	1.00	69.41	B
5398	CA	SER	B1218	8.954	31.992	4.956	1.00	69.34	B
5399	CB	SER	B1218	7.869	32.461	3.977	1.00	70.69	B
5400	OG	SER	B1218	7.155	31.266	3.526	1.00	64.46	B
5401	C	SER	B1218	9.556	30.879	4.225	1.00	69.87	B
5402	O	SER	B1218	9.981	31.052	3.069	1.00	69.54	B
5403	N	GLY	B1219	9.527	29.734	4.917	1.00	69.51	B
5404	CA	GLY	B1219	10.043	28.516	4.383	1.00	66.93	B
5405	C	GLY	B1219	11.538	28.520	4.707	1.00	64.85	B
5406	O	GLY	B1219	12.110	27.456	4.928	1.00	67.53	B
5407	N	LYS	B1220	12.226	29.652	4.727	1.00	61.90	B
5408	CA	LYS	B1220	13.706	29.565	5.060	1.00	60.24	B
5409	CB	LYS	B1220	14.605	29.835	3.823	1.00	56.47	B
5410	CG	LYS	B1220	13.765	29.325	2.459	1.00	54.40	B
5411	CD	LYS	B1220	14.812	28.591	1.458	1.00	55.73	B
5412	CE	LYS	B1220	14.662	28.817	-0.092	1.00	44.67	B
5413	NZ	LYS	B1220	16.103	28.789	-0.758	1.00	41.31	B
5414	C	LYS	B1220	14.244	30.076	6.489	1.00	61.77	B
5415	O	LYS	B1220	13.517	30.424	7.441	1.00	59.14	B
5416	N	VAL	B1221	15.535	29.870	6.662	1.00	62.06	B
5417	CA	VAL	B1221	16.215	30.646	7.568	1.00	61.04	B
5418	CB	VAL	B1221	16.791	29.810	8.619	1.00	61.71	B
5419	CG1	VAL	B1221	17.029	28.515	8.081	1.00	64.97	B

5420	CG2	VAL	B1221	18.105	30.439	9.225	1.00	63.56	B
5421	C	VAL	B1221	17.251	31.253	6.718	1.00	59.72	B
5422	O	VAL	B1221	17.954	30.561	5.990	1.00	55.38	B
5423	N	ALA	B1222	17.172	32.588	6.730	1.00	62.54	B
5424	CA	ALA	B1222	18.310	33.563	6.549	1.00	63.67	B
5425	CB	ALA	B1222	17.939	34.850	5.694	1.00	61.50	B
5426	C	ALA	B1222	18.819	33.955	7.976	1.00	64.35	B
5427	O	ALA	B1222	18.155	34.694	8.799	1.00	63.55	B
5428	N	PHE	B1223	20.045	33.444	8.173	1.00	63.98	B
5429	CA	PHE	B1223	20.964	33.668	9.289	1.00	61.74	B
5430	CB	PHE	B1223	22.242	32.817	9.060	1.00	60.54	B
5431	CG	PHE	B1223	22.002	31.369	8.870	1.00	57.18	B
5432	CD1	PHE	B1223	21.004	30.664	9.637	1.00	56.35	B
5433	CD2	PHE	B1223	22.759	30.653	7.899	1.00	61.33	B
5434	CE1	PHE	B1223	20.791	29.239	9.471	1.00	57.87	B
5435	CE2	PHE	B1223	22.560	29.129	7.713	1.00	59.65	B
5436	CZ	PHE	B1223	21.580	28.460	8.493	1.00	54.24	B
5437	C	PHE	B1223	21.495	35.003	9.411	1.00	61.59	B
5438	O	PHE	B1223	22.263	35.394	8.503	1.00	62.01	B
5439	N	ARG	B1224	21.222	35.676	10.543	1.00	61.72	B
5440	CA	ARG	B1224	22.027	36.850	10.888	1.00	62.11	B
5441	CB	ARG	B1224	21.572	37.458	12.103	1.00	60.10	B
5442	CG	ARG	B1224	20.979	38.768	11.866	1.00	66.66	B
5443	CD	ARG	B1224	21.987	39.902	11.497	1.00	75.37	B
5444	NE	ARG	B1224	21.385	41.109	10.832	1.00	74.00	B
5445	CZ	ARG	B1224	21.262	42.315	11.393	1.00	72.34	B
5446	NH1	ARG	B1224	21.648	42.608	12.644	1.00	68.75	B
5447	NH2	ARG	B1224	20.776	43.263	10.662	1.00	77.74	B
5448	C	ARG	B1224	23.463	36.496	11.138	1.00	64.13	B
5449	O	ARG	B1224	23.830	35.341	11.321	1.00	63.37	B
5450	N	ASP	B1225	24.311	37.525	11.125	1.00	67.32	B
5451	CA	ASP	B1225	25.705	37.417	11.582	1.00	68.20	B
5452	CB	ASP	B1225	26.749	37.228	10.464	1.00	68.95	B
5453	CG	ASP	B1225	27.579	38.547	10.064	1.00	73.18	B
5454	OD1	ASP	B1225	28.053	39.287	10.984	1.00	75.85	B
5455	OD2	ASP	B1225	27.849	38.757	8.812	1.00	70.10	B
5456	C	ASP	B1225	25.912	38.615	12.351	1.00	69.73	B
5457	O	ASP	B1225	25.271	39.663	12.120	1.00	71.24	B
5458	N	CYS	B1226	26.843	38.442	13.251	1.00	72.12	B
5459	CA	CYS	B1226	27.162	39.354	14.345	1.00	75.96	B
5460	CB	CYS	B1226	28.003	38.574	15.483	1.00	76.99	B
5461	SG	CYS	B1226	29.531	37.606	14.929	1.00	77.47	B
5462	C	CYS	B1226	27.833	40.680	13.943	1.00	74.83	B
5463	O	CYS	B1226	28.492	41.346	14.776	1.00	75.32	B
5464	N	GLU	B1227	27.705	40.988	12.667	1.00	75.01	B
5465	CA	GLU	B1227	28.210	42.205	12.070	1.00	75.65	B
5466	CB	GLU	B1227	29.178	41.846	10.939	1.00	73.43	B
5467	CG	GLU	B1227	30.603	41.316	11.346	1.00	73.46	B
5468	CD	GLU	B1227	31.444	42.335	12.217	1.00	75.42	B
5469	OE1	GLU	B1227	32.717	42.404	12.012	1.00	73.44	B
5470	OE2	GLU	B1227	30.836	43.048	13.099	1.00	68.23	B
5471	C	GLU	B1227	27.003	43.139	11.588	1.00	77.70	B
5472	O	GLU	B1227	27.195	44.237	11.005	1.00	80.30	B
5473	N	GLY	B1228	25.754	42.752	11.838	1.00	77.00	B
5474	CA	GLY	B1228	24.699	43.254	10.951	1.00	75.83	B
5475	C	GLY	B1228	24.705	42.548	9.551	1.00	75.08	B

5476	O	GLY	B1228	23.647	42.444	8.837	1.00	72.10	B
5477	N	ARG	B1229	25.900	42.071	9.157	1.00	74.97	B
5478	CA	ARG	B1229	26.034	41.274	7.895	1.00	74.64	B
5479	CB	ARG	B1229	27.538	41.134	7.475	1.00	75.05	B
5480	CG	ARG	B1229	27.963	41.953	6.241	1.00	73.86	B
5481	CD	ARG	B1229	29.091	43.033	6.383	1.00	68.40	B
5482	NE	ARG	B1229	30.151	42.892	7.417	1.00	74.54	B
5483	CZ	ARG	B1229	31.446	42.464	7.320	1.00	76.47	B
5484	NH1	ARG	B1229	31.954	42.011	6.142	1.00	78.34	B
5485	NH2	ARG	B1229	32.285	42.469	8.431	1.00	65.02	B
5486	C	ARG	B1229	25.201	39.919	8.018	1.00	72.97	B
5487	O	ARG	B1229	24.358	39.762	8.971	1.00	76.06	B
5488	N	TYR	B1230	25.369	38.998	7.093	1.00	68.22	B
5489	CA	TYR	B1230	24.412	37.922	6.923	1.00	66.47	B
5490	CB	TYR	B1230	23.118	38.304	6.120	1.00	65.13	B
5491	CG	TYR	B1230	21.950	39.143	6.583	1.00	58.96	B
5492	CD1	TYR	B1230	21.998	40.480	6.603	1.00	53.96	B
5493	CE1	TYR	B1230	20.693	41.329	6.963	1.00	63.45	B
5494	CD2	TYR	B1230	20.680	38.543	6.787	1.00	63.41	B
5495	CE2	TYR	B1230	19.386	39.301	7.071	1.00	58.78	B
5496	CZ	TYR	B1230	19.409	40.668	7.150	1.00	64.14	B
5497	OH	TYR	B1230	18.196	41.340	7.463	1.00	63.39	B
5498	C	TYR	B1230	25.189	36.999	5.981	1.00	66.58	B
5499	O	TYR	B1230	25.765	37.483	5.008	1.00	63.48	B
5500	N	LEU	B1231	25.144	35.691	6.287	1.00	67.86	B
5501	CA	LEU	B1231	26.003	34.603	5.740	1.00	69.53	B
5502	CB	LEU	B1231	26.298	33.560	6.897	1.00	68.55	B
5503	CG	LEU	B1231	27.496	33.812	7.912	1.00	68.20	B
5504	CD1	LEU	B1231	27.121	33.771	9.492	1.00	60.77	B
5505	CD2	LEU	B1231	28.908	32.961	7.653	1.00	61.08	B
5506	C	LEU	B1231	25.547	33.904	4.356	1.00	69.56	B
5507	O	LEU	B1231	24.344	33.737	4.128	1.00	71.79	B
5508	N	ALA	B1232	26.452	33.438	3.476	1.00	67.19	B
5509	CA	ALA	B1232	25.971	33.071	2.160	1.00	66.38	B
5510	CB	ALA	B1232	25.319	34.348	1.460	1.00	66.64	B
5511	C	ALA	B1232	27.026	32.424	1.255	1.00	66.57	B
5512	O	ALA	B1232	28.233	32.868	1.237	1.00	65.57	B
5513	N	PRO	B1233	26.593	31.378	0.456	1.00	66.30	B
5514	CD	PRO	B1233	25.254	30.760	0.445	1.00	64.69	B
5515	CA	PRO	B1233	27.424	30.749	-0.619	1.00	65.82	B
5516	CB	PRO	B1233	26.354	30.429	-1.635	1.00	65.13	B
5517	CG	PRO	B1233	25.265	29.904	-0.787	1.00	62.08	B
5518	C	PRO	B1233	28.493	31.704	-1.261	1.00	65.95	B
5519	O	PRO	B1233	28.137	32.809	-1.470	1.00	67.40	B
5520	N	SER	B1234	29.762	31.293	-1.452	1.00	65.61	B
5521	CA	SER	B1234	30.860	31.971	-2.167	1.00	63.45	B
5522	CB	SER	B1234	32.077	32.063	-1.246	1.00	63.22	B
5523	OG	SER	B1234	33.301	32.364	-1.952	1.00	62.69	B
5524	C	SER	B1234	31.314	31.080	-3.399	1.00	63.92	B
5525	O	SER	B1234	30.460	30.609	-4.202	1.00	62.01	B
5526	N	GLY	B1235	32.655	30.885	-3.530	1.00	61.90	B
5527	CA	GLY	B1235	33.252	29.749	-4.265	1.00	59.42	B
5528	C	GLY	B1235	32.316	28.878	-5.062	1.00	56.69	B
5529	O	GLY	B1235	31.159	29.181	-5.143	1.00	52.94	B
5530	N	PRO	B1236	32.873	27.905	-5.808	1.00	58.47	B
5531	CD	PRO	B1236	34.144	28.108	-6.543	1.00	60.27	B

5532	CA	PRO	B1236	32.281	26.591	-6.170	1.00	59.57	B
5533	CB	PRO	B1236	33.271	26.025	-7.235	1.00	61.04	B
5534	CG	PRO	B1236	33.976	27.230	-7.809	1.00	59.35	B
5535	C	PRO	B1236	32.290	25.658	-4.953	1.00	60.59	B
5536	O	PRO	B1236	31.689	24.520	-5.020	1.00	57.74	B
5537	N	SER	B1237	33.018	26.122	-3.880	1.00	61.47	B
5538	CA	SER	B1237	33.140	25.320	-2.665	1.00	62.54	B
5539	CB	SER	B1237	34.569	25.212	-2.004	1.00	61.62	B
5540	OG	SER	B1237	35.288	26.456	-1.878	1.00	63.60	B
5541	C	SER	B1237	32.055	25.923	-1.855	1.00	62.28	B
5542	O	SER	B1237	31.995	25.790	-0.642	1.00	67.38	B
5543	N	GLY	B1238	31.091	26.495	-2.542	1.00	61.04	B
5544	CA	GLY	B1238	30.084	27.354	-1.860	1.00	61.43	B
5545	C	GLY	B1238	30.634	27.890	-0.511	1.00	60.43	B
5546	O	GLY	B1238	29.957	27.886	0.476	1.00	58.97	B
5547	N	THR	B1239	31.891	28.295	-0.461	1.00	59.86	B
5548	CA	THR	B1239	32.466	28.610	0.888	1.00	61.17	B
5549	CB	THR	B1239	33.977	29.181	0.763	1.00	63.48	B
5550	OG1	THR	B1239	34.681	28.731	-0.505	1.00	60.75	B
5551	CG2	THR	B1239	34.810	29.051	2.253	1.00	60.50	B
5552	C	THR	B1239	31.561	29.595	1.770	1.00	59.30	B
5553	O	THR	B1239	31.582	30.771	1.675	1.00	59.26	B
5554	N	LEU	B1240	30.696	29.114	2.571	1.00	58.94	B
5555	CA	LEU	B1240	29.931	30.026	3.331	1.00	61.17	B
5556	CB	LEU	B1240	28.781	29.231	3.954	1.00	60.08	B
5557	CG	LEU	B1240	28.791	27.843	3.348	1.00	56.94	B
5558	CD1	LEU	B1240	28.241	26.789	4.342	1.00	50.19	B
5559	CD2	LEU	B1240	28.018	27.923	1.984	1.00	64.18	B
5560	C	LEU	B1240	30.774	30.735	4.454	1.00	62.94	B
5561	O	LEU	B1240	31.492	30.018	5.273	1.00	66.34	B
5562	N	LYS	B1244	28.212	40.485	3.577	1.00	71.54	B
5563	CA	LYS	B1244	28.266	41.794	3.000	1.00	72.69	B
5564	CB	LYS	B1244	29.449	42.010	2.040	1.00	73.46	B
5565	CG	LYS	B1244	29.906	40.799	1.068	1.00	73.56	B
5566	CD	LYS	B1244	31.267	41.254	0.301	1.00	74.39	B
5567	CE	LYS	B1244	32.662	41.018	1.191	1.00	71.86	B
5568	NZ	LYS	B1244	33.638	42.140	0.863	1.00	68.59	B
5569	C	LYS	B1244	26.931	41.906	2.332	1.00	73.62	B
5570	O	LYS	B1244	26.795	41.800	1.052	1.00	76.06	B
5571	N	ALA	B1245	25.908	42.021	3.195	1.00	71.23	B
5572	CA	ALA	B1245	24.574	42.056	2.683	1.00	68.40	B
5573	CB	ALA	B1245	23.916	40.619	2.725	1.00	68.20	B
5574	C	ALA	B1245	23.773	43.053	3.487	1.00	67.74	B
5575	O	ALA	B1245	23.660	42.952	4.770	1.00	67.65	B
5576	N	THR	B1246	23.202	44.012	2.755	1.00	65.07	B
5577	CA	THR	B1246	22.270	44.929	3.387	1.00	62.60	B
5578	CB	THR	B1246	22.001	46.266	2.532	1.00	61.77	B
5579	OG1	THR	B1246	23.188	46.604	1.788	1.00	55.70	B
5580	CG2	THR	B1246	21.534	47.455	3.428	1.00	60.20	B
5581	C	THR	B1246	21.028	44.079	3.644	1.00	62.40	B
5582	O	THR	B1246	20.920	43.487	4.751	1.00	63.06	B
5583	N	LYS	B1247	20.124	44.036	2.642	1.00	61.22	B
5584	CA	LYS	B1247	18.801	43.446	2.816	1.00	60.96	B
5585	CB	LYS	B1247	17.713	44.099	1.974	1.00	60.47	B
5586	CG	LYS	B1247	16.298	43.438	2.261	1.00	54.10	B
5587	CD	LYS	B1247	15.279	44.487	2.409	1.00	54.54	B

5588	CE	LYS	B1247	15.701	45.979	2.022	1.00	48.70	B
5589	NZ	LYS	B1247	14.519	46.912	1.754	1.00	43.98	B
5590	C	LYS	B1247	18.962	42.007	2.461	1.00	61.67	B
5591	O	LYS	B1247	19.885	41.726	1.709	1.00	60.26	B
5592	N	VAL	B1248	18.163	41.107	3.100	1.00	63.43	B
5593	CA	VAL	B1248	18.139	39.638	2.698	1.00	63.99	B
5594	CB	VAL	B1248	17.021	38.806	3.547	1.00	62.13	B
5595	CG1	VAL	B1248	15.560	38.940	3.015	1.00	65.30	B
5596	CG2	VAL	B1248	17.291	37.444	3.574	1.00	54.18	B
5597	C	VAL	B1248	17.988	39.601	1.093	1.00	65.09	B
5598	O	VAL	B1248	17.047	40.234	0.502	1.00	65.84	B
5599	N	GLY	B1249	18.918	38.927	0.406	1.00	66.31	B
5600	CA	GLY	B1249	18.983	38.836	-1.121	1.00	65.33	B
5601	C	GLY	B1249	18.460	37.423	-1.473	1.00	67.14	B
5602	O	GLY	B1249	17.886	36.695	-0.614	1.00	67.68	B
5603	N	LYS	B1250	18.641	37.013	-2.713	1.00	66.62	B
5604	CA	LYS	B1250	18.063	35.818	-3.208	1.00	64.94	B
5605	CB	LYS	B1250	18.130	35.906	-4.718	1.00	66.64	B
5606	CG	LYS	B1250	19.302	36.895	-5.404	1.00	64.78	B
5607	CD	LYS	B1250	19.153	36.798	-7.008	1.00	58.62	B
5608	CE	LYS	B1250	18.009	37.636	-7.595	1.00	50.08	B
5609	NZ	LYS	B1250	16.681	36.811	-7.687	1.00	49.90	B
5610	C	LYS	B1250	18.835	34.506	-2.754	1.00	67.65	B
5611	O	LYS	B1250	18.258	33.381	-2.851	1.00	65.76	B
5612	N	ASP	B1251	20.125	34.661	-2.349	1.00	67.20	B
5613	CA	ASP	B1251	20.983	33.578	-1.766	1.00	67.10	B
5614	CB	ASP	B1251	22.468	33.891	-1.998	1.00	69.09	B
5615	CG	ASP	B1251	22.699	35.420	-2.355	1.00	74.14	B
5616	OD1	ASP	B1251	22.685	35.850	-3.569	1.00	75.10	B
5617	OD2	ASP	B1251	22.860	36.207	-1.378	1.00	80.61	B
5618	C	ASP	B1251	20.773	33.240	-0.273	1.00	65.83	B
5619	O	ASP	B1251	20.271	32.145	0.053	1.00	62.43	B
5620	N	GLU	B1252	21.208	34.177	0.584	1.00	65.16	B
5621	CA	GLU	B1252	21.265	34.111	2.100	1.00	65.85	B
5622	CB	GLU	B1252	21.003	35.513	2.687	1.00	63.70	B
5623	CG	GLU	B1252	22.062	36.623	2.461	1.00	71.12	B
5624	CD	GLU	B1252	21.893	37.336	1.079	1.00	74.74	B
5625	OE1	GLU	B1252	22.394	38.469	0.939	1.00	71.11	B
5626	OE2	GLU	B1252	21.219	36.763	0.144	1.00	78.95	B
5627	C	GLU	B1252	20.371	33.155	2.980	1.00	65.26	B
5628	O	GLU	B1252	20.498	33.196	4.223	1.00	65.50	B
5629	N	LEU	B1253	19.483	32.381	2.329	1.00	63.81	B
5630	CA	LEU	B1253	18.240	31.829	2.855	1.00	63.61	B
5631	CB	LEU	B1253	17.064	32.060	1.853	1.00	62.78	B
5632	CG	LEU	B1253	15.941	33.065	1.522	1.00	62.78	B
5633	CD1	LEU	B1253	14.670	33.031	2.498	1.00	68.28	B
5634	CD2	LEU	B1253	16.380	34.575	1.253	1.00	63.71	B
5635	C	LEU	B1253	18.477	30.335	2.853	1.00	63.79	B
5636	O	LEU	B1253	18.784	29.783	1.804	1.00	65.56	B
5637	N	PHE	B1254	18.311	29.638	3.964	1.00	64.25	B
5638	CA	PHE	B1254	18.765	28.231	3.967	1.00	65.04	B
5639	CB	PHE	B1254	19.896	28.068	4.959	1.00	63.16	B
5640	CG	PHE	B1254	21.316	28.453	4.381	1.00	69.08	B
5641	CD1	PHE	B1254	21.756	27.966	3.081	1.00	64.84	B
5642	CD2	PHE	B1254	22.220	29.354	5.148	1.00	64.20	B
5643	CE1	PHE	B1254	23.071	28.342	2.574	1.00	63.94	B

5644	CE2	PHE	B1254	23.558	29.693	4.663	1.00	57.66	B
5645	CZ	PHE	B1254	24.006	29.189	3.406	1.00	57.11	B
5646	C	PHE	B1254	17.651	27.179	4.198	1.00	66.15	B
5647	O	PHE	B1254	16.690	27.430	5.001	1.00	68.23	B
5648	N	ALA	B1255	17.721	26.042	3.472	1.00	64.52	B
5649	CA	ALA	B1255	16.832	24.915	3.734	1.00	60.37	B
5650	CB	ALA	B1255	16.942	24.015	2.605	1.00	62.62	B
5651	C	ALA	B1255	17.439	24.233	4.887	1.00	59.50	B
5652	O	ALA	B1255	18.594	23.825	4.784	1.00	60.72	B
5653	N	LEU	B1256	16.688	24.063	5.961	1.00	58.16	B
5654	CA	LEU	B1256	17.099	23.335	7.173	1.00	55.49	B
5655	CB	LEU	B1256	16.719	24.123	8.465	1.00	53.65	B
5656	CG	LEU	B1256	17.673	25.374	8.586	1.00	52.33	B
5657	CD1	LEU	B1256	17.382	26.394	9.879	1.00	43.49	B
5658	CD2	LEU	B1256	19.156	25.059	8.315	1.00	40.69	B
5659	C	LEU	B1256	16.374	22.037	7.180	1.00	54.68	B
5660	O	LEU	B1256	15.230	22.024	7.634	1.00	54.86	B
5661	N	GLU	B1257	16.990	20.944	6.698	1.00	55.28	B
5662	CA	GLU	B1257	16.331	19.572	6.836	1.00	55.55	B
5663	CB	GLU	B1257	16.379	18.812	5.561	1.00	56.54	B
5664	CG	GLU	B1257	17.517	19.171	4.759	1.00	58.88	B
5665	CD	GLU	B1257	17.140	19.206	3.343	1.00	64.12	B
5666	OE1	GLU	B1257	17.932	18.460	2.694	1.00	66.73	B
5667	OE2	GLU	B1257	16.107	19.927	2.938	1.00	55.38	B
5668	C	GLU	B1257	16.829	18.598	7.936	1.00	55.93	B
5669	O	GLU	B1257	18.040	18.523	8.141	1.00	57.66	B
5670	N	GLN	B1258	15.906	17.913	8.635	1.00	53.64	B
5671	CA	GLN	B1258	16.198	16.780	9.430	1.00	53.86	B
5672	CB	GLN	B1258	14.921	15.951	9.661	1.00	53.27	B
5673	CG	GLN	B1258	13.725	16.759	10.247	1.00	54.42	B
5674	CD	GLN	B1258	12.444	16.035	10.588	1.00	52.44	B
5675	OE1	GLN	B1258	11.453	16.708	10.883	1.00	54.92	B
5676	NE2	GLN	B1258	12.412	14.711	10.477	1.00	48.80	B
5677	C	GLN	B1258	17.282	15.937	8.751	1.00	55.40	B
5678	O	GLN	B1258	17.224	15.579	7.551	1.00	56.48	B
5679	N	SER	B1259	18.316	15.633	9.533	1.00	56.27	B
5680	CA	SER	B1259	19.370	14.653	9.156	1.00	53.65	B
5681	CB	SER	B1259	20.595	15.057	9.896	1.00	55.96	B
5682	OG	SER	B1259	21.247	13.921	10.140	1.00	60.48	B
5683	C	SER	B1259	18.959	13.350	9.691	1.00	50.46	B
5684	O	SER	B1259	18.457	13.272	10.809	1.00	48.82	B
5685	N	CYS	B1260	19.137	12.302	8.912	1.00	50.46	B
5686	CA	CYS	B1260	18.695	10.952	9.416	1.00	51.51	B
5687	CB	CYS	B1260	17.747	10.151	8.490	1.00	53.28	B
5688	SG	CYS	B1260	16.107	10.795	8.181	1.00	50.55	B
5689	C	CYS	B1260	19.897	10.125	9.805	1.00	48.69	B
5690	O	CYS	B1260	20.947	10.357	9.198	1.00	47.86	B
5691	N	ALA	B1261	19.762	9.350	10.865	1.00	43.86	B
5692	CA	ALA	B1261	20.682	8.184	11.037	1.00	46.63	B
5693	CB	ALA	B1261	20.166	7.075	12.163	1.00	45.05	B
5694	C	ALA	B1261	21.154	7.394	9.782	1.00	48.10	B
5695	O	ALA	B1261	20.352	7.003	8.843	1.00	47.89	B
5696	N	GLN	B1262	22.481	7.160	9.811	1.00	47.86	B
5697	CA	GLN	B1262	23.166	6.604	8.693	1.00	50.13	B
5698	CB	GLN	B1262	23.987	7.695	7.842	1.00	48.76	B
5699	CG	GLN	B1262	23.055	8.721	7.171	1.00	45.44	B

5700	CD	GLN	B1262	23.644	9.723	6.078	1.00	48.23	B
5701	OE1	GLN	B1262	24.859	9.974	6.012	1.00	45.91	B
5702	NE2	GLN	B1262	22.733	10.279	5.209	1.00	38.52	B
5703	C	GLN	B1262	23.976	5.522	9.375	1.00	50.73	B
5704	O	GLN	B1262	24.649	5.750	10.395	1.00	51.73	B
5705	N	VAL	B1263	23.796	4.311	8.852	1.00	51.73	B
5706	CA	VAL	B1263	24.424	3.101	9.399	1.00	49.38	B
5707	CB	VAL	B1263	23.439	2.282	10.236	1.00	47.37	B
5708	CG1	VAL	B1263	22.574	3.162	11.042	1.00	45.25	B
5709	CG2	VAL	B1263	22.491	1.495	9.423	1.00	50.88	B
5710	C	VAL	B1263	25.003	2.449	8.165	1.00	50.25	B
5711	O	VAL	B1263	24.552	2.806	7.037	1.00	47.08	B
5712	N	VAL	B1264	26.197	1.907	8.421	1.00	52.80	B
5713	CA	VAL	B1264	26.835	0.638	7.948	1.00	57.04	B
5714	CB	VAL	B1264	28.213	0.541	8.739	1.00	55.28	B
5715	CG1	VAL	B1264	28.906	-0.789	8.684	1.00	56.13	B
5716	CG2	VAL	B1264	29.156	1.649	8.480	1.00	52.61	B
5717	C	VAL	B1264	26.017	-0.597	8.499	1.00	59.69	B
5718	O	VAL	B1264	25.599	-0.541	9.679	1.00	64.42	B
5719	N	LEU	B1265	25.824	-1.709	7.791	1.00	60.48	B
5720	CA	LEU	B1265	25.165	-2.976	8.421	1.00	60.28	B
5721	CB	LEU	B1265	23.955	-3.519	7.645	1.00	59.22	B
5722	CG	LEU	B1265	22.540	-2.943	7.904	1.00	60.86	B
5723	CD1	LEU	B1265	21.596	-3.668	6.986	1.00	63.25	B
5724	CD2	LEU	B1265	21.998	-3.014	9.297	1.00	54.48	B
5725	C	LEU	B1265	26.020	-4.163	8.272	1.00	61.83	B
5726	O	LEU	B1265	26.029	-4.641	7.151	1.00	62.59	B
5727	N	GLN	B1266	26.681	-4.677	9.333	1.00	62.80	B
5728	CA	GLN	B1266	27.644	-5.815	9.191	1.00	61.55	B
5729	CB	GLN	B1266	28.546	-5.888	10.383	1.00	59.62	B
5730	CG	GLN	B1266	29.874	-6.582	10.166	1.00	61.70	B
5731	CD	GLN	B1266	31.046	-5.544	10.129	1.00	66.97	B
5732	OE1	GLN	B1266	31.199	-4.709	11.055	1.00	69.42	B
5733	NE2	GLN	B1266	31.801	-5.526	9.023	1.00	63.64	B
5734	C	GLN	B1266	26.765	-7.085	9.150	1.00	63.45	B
5735	O	GLN	B1266	25.654	-7.051	9.698	1.00	63.56	B
5736	N	ALA	B1267	27.193	-8.161	8.439	1.00	63.25	B
5737	CA	ALA	B1267	26.512	-9.468	8.505	1.00	63.41	B
5738	CB	ALA	B1267	26.341	-10.120	7.149	1.00	61.94	B
5739	C	ALA	B1267	27.208	-10.430	9.484	1.00	65.04	B
5740	O	ALA	B1267	28.278	-10.110	10.118	1.00	61.86	B
5741	N	ALA	B1268	26.564	-11.596	9.650	1.00	67.06	B
5742	CA	ALA	B1268	27.358	-12.748	10.078	1.00	70.33	B
5743	CB	ALA	B1268	26.537	-13.972	9.937	1.00	67.92	B
5744	C	ALA	B1268	28.769	-12.837	9.337	1.00	71.63	B
5745	O	ALA	B1268	29.803	-12.360	9.880	1.00	71.81	B
5746	N	ASN	B1269	28.820	-13.386	8.091	1.00	74.31	B
5747	CA	ASN	B1269	30.144	-13.672	7.399	1.00	75.37	B
5748	CB	ASN	B1269	30.109	-13.407	5.877	1.00	75.03	B
5749	CG	ASN	B1269	30.150	-11.815	5.509	1.00	78.73	B
5750	OD1	ASN	B1269	30.686	-11.380	4.451	1.00	86.70	B
5751	ND2	ASN	B1269	29.582	-10.982	6.381	1.00	72.30	B
5752	C	ASN	B1269	31.010	-12.592	7.901	1.00	78.47	B
5753	O	ASN	B1269	32.208	-12.747	8.440	1.00	78.18	B
5754	N	GLU	B1270	30.411	-11.403	7.543	1.00	80.00	B
5755	CA	GLU	B1270	30.899	-10.087	7.872	1.00	81.75	B

5756	CB	GLU	B1270	32.429	-10.175	8.172	1.00	84.61	B
5757	CG	GLU	B1270	32.700	-11.123	9.373	1.00	88.89	B
5758	CD	GLU	B1270	31.781	-10.595	10.406	1.00	95.74	B
5759	OE1	GLU	B1270	31.619	-9.258	10.327	1.00	100.59	B
5760	OE2	GLU	B1270	31.201	-11.445	11.159	1.00	98.48	B
5761	C	GLU	B1270	30.641	-9.291	6.669	1.00	80.54	B
5762	O	GLU	B1270	30.654	-8.220	5.839	1.00	84.03	B
5763	N	ARG	B1271	31.483	-8.652	7.519	1.00	77.88	B
5764	CA	ARG	B1271	31.989	-7.472	6.904	1.00	74.73	B
5765	CB	ARG	B1271	32.711	-7.900	5.523	1.00	75.80	B
5766	CG	ARG	B1271	33.175	-9.438	5.302	1.00	76.27	B
5767	CD	ARG	B1271	34.769	-9.628	5.251	1.00	78.76	B
5768	NE	ARG	B1271	35.338	-8.874	4.139	1.00	76.25	B
5769	CZ	ARG	B1271	35.026	-9.088	2.868	1.00	77.11	B
5770	NH1	ARG	B1271	34.157	-10.081	2.494	1.00	79.02	B
5771	NH2	ARG	B1271	35.586	-8.287	1.961	1.00	74.65	B
5772	C	ARG	B1271	30.555	-6.762	6.668	1.00	71.80	B
5773	O	ARG	B1271	29.433	-7.278	7.088	1.00	69.22	B
5774	N	ASN	B1272	30.565	-5.619	6.005	1.00	69.67	B
5775	CA	ASN	B1272	29.276	-4.811	5.944	1.00	69.77	B
5776	CB	ASN	B1272	29.630	-3.388	6.351	1.00	67.42	B
5777	CG	ASN	B1272	31.086	-3.242	6.514	1.00	64.07	B
5778	OD1	ASN	B1272	31.689	-3.700	7.476	1.00	57.97	B
5779	ND2	ASN	B1272	31.684	-2.650	5.524	1.00	62.13	B
5780	C	ASN	B1272	28.450	-4.957	4.607	1.00	65.32	B
5781	O	ASN	B1272	29.029	-5.348	3.657	1.00	67.35	B
5782	N	VAL	B1273	27.125	-4.825	4.538	1.00	61.88	B
5783	CA	VAL	B1273	26.542	-4.789	3.182	1.00	59.48	B
5784	CB	VAL	B1273	25.064	-4.694	3.153	1.00	58.14	B
5785	CG1	VAL	B1273	24.439	-5.635	4.097	1.00	60.12	B
5786	CG2	VAL	B1273	24.726	-3.375	3.608	1.00	61.27	B
5787	C	VAL	B1273	26.995	-3.485	2.509	1.00	59.21	B
5788	O	VAL	B1273	26.943	-2.398	3.149	1.00	60.51	B
5789	N	SER	B1274	27.445	-3.604	1.259	1.00	56.06	B
5790	CA	SER	B1274	27.812	-2.492	0.440	1.00	55.05	B
5791	CB	SER	B1274	29.304	-2.453	0.076	1.00	58.00	B
5792	OG	SER	B1274	29.531	-1.172	-0.514	1.00	55.32	B
5793	C	SER	B1274	27.092	-2.517	-0.809	1.00	52.98	B
5794	O	SER	B1274	26.754	-3.546	-1.232	1.00	52.31	B
5795	N	GLY	B1275	26.906	-1.376	-1.432	1.00	53.75	B
5796	CA	GLY	B1275	26.100	-1.304	-2.718	1.00	55.78	B
5797	C	GLY	B1275	27.051	-1.037	-3.856	1.00	56.35	B
5798	O	GLY	B1275	26.764	-1.366	-4.915	1.00	57.09	B
5799	N	ARG	B1276	28.168	-0.385	-3.559	1.00	60.47	B
5800	CA	ARG	B1276	29.356	-0.081	-4.356	1.00	62.99	B
5801	CB	ARG	B1276	30.646	0.155	-3.483	1.00	61.78	B
5802	CG	ARG	B1276	32.081	-0.054	-4.226	1.00	64.88	B
5803	CD	ARG	B1276	33.617	-0.057	-3.433	1.00	63.61	B
5804	NE	ARG	B1276	33.585	-0.209	-1.972	1.00	73.76	B
5805	CZ	ARG	B1276	34.639	-0.376	-1.112	1.00	73.49	B
5806	NH1	ARG	B1276	35.941	-0.495	-1.583	1.00	65.99	B
5807	NH2	ARG	B1276	34.359	-0.367	0.262	1.00	58.56	B
5808	C	ARG	B1276	29.486	-1.265	-5.263	1.00	66.64	B
5809	O	ARG	B1276	29.072	-2.411	-4.892	1.00	68.09	B
5810	N	GLN	B1277	30.002	-0.991	-6.479	1.00	68.87	B
5811	CA	GLN	B1277	29.961	-1.958	-7.541	1.00	68.86	B

5812	CB	GLN	B1277	30.762	-3.299	-7.126	1.00	68.84	B
5813	CG	GLN	B1277	32.474	-3.241	-7.186	1.00	71.51	B
5814	CD	GLN	B1277	33.338	-4.300	-6.198	1.00	69.82	B
5815	OE1	GLN	B1277	34.167	-5.077	-6.667	1.00	58.11	B
5816	NE2	GLN	B1277	33.128	-4.236	-4.867	1.00	73.00	B
5817	C	GLN	B1277	28.439	-2.065	-7.576	1.00	68.32	B
5818	O	GLN	B1277	27.852	-3.086	-7.159	1.00	69.00	B
5819	N	THR	B1278	27.711	-1.024	-7.948	1.00	68.13	B
5820	CA	THR	B1278	26.206	-1.385	-7.851	1.00	71.38	B
5821	CB	THR	B1278	25.166	-0.209	-7.549	1.00	69.54	B
5822	OG1	THR	B1278	23.852	-0.781	-7.413	1.00	71.32	B
5823	CG2	THR	B1278	25.160	0.745	-8.586	1.00	68.49	B
5824	C	THR	B1278	25.532	-2.592	-8.697	1.00	72.13	B
5825	O	THR	B1278	26.108	-3.135	-9.696	1.00	72.64	B
5826	N	MET	B1279	24.342	-3.020	-8.218	1.00	72.69	B
5827	CA	MET	B1279	23.723	-4.302	-8.613	1.00	71.98	B
5828	CB	MET	B1279	24.792	-5.317	-8.904	1.00	70.74	B
5829	CG	MET	B1279	24.726	-5.708	-10.280	1.00	72.54	B
5830	SD	MET	B1279	23.055	-5.572	-11.137	1.00	68.45	B
5831	CE	MET	B1279	22.300	-7.264	-10.604	1.00	67.93	B
5832	C	MET	B1279	22.796	-5.051	-7.666	1.00	73.09	B
5833	O	MET	B1279	22.065	-5.928	-8.177	1.00	73.93	B
5834	N	ASP	B1280	22.861	-4.786	-6.330	1.00	72.16	B
5835	CA	ASP	B1280	22.240	-5.626	-5.349	1.00	71.16	B
5836	CB	ASP	B1280	22.334	-7.113	-5.757	1.00	69.94	B
5837	CG	ASP	B1280	22.826	-7.985	-4.597	1.00	65.20	B
5838	OD1	ASP	B1280	22.219	-7.944	-3.509	1.00	63.82	B
5839	OD2	ASP	B1280	23.867	-8.603	-4.718	1.00	61.36	B
5840	C	ASP	B1280	23.037	-5.570	-4.038	1.00	74.06	B
5841	O	ASP	B1280	24.316	-5.785	-4.044	1.00	74.60	B
5842	N	LEU	B1281	22.273	-5.502	-2.905	1.00	74.36	B
5843	CA	LEU	B1281	22.873	-5.411	-1.556	1.00	73.55	B
5844	CB	LEU	B1281	21.879	-4.847	-0.555	1.00	72.93	B
5845	CG	LEU	B1281	21.170	-3.773	-1.354	1.00	72.10	B
5846	CD1	LEU	B1281	19.664	-3.663	-1.057	1.00	75.52	B
5847	CD2	LEU	B1281	21.893	-2.456	-1.254	1.00	75.77	B
5848	C	LEU	B1281	23.357	-6.797	-1.236	1.00	73.52	B
5849	O	LEU	B1281	22.552	-7.807	-1.347	1.00	75.21	B
5850	N	SER	B1282	24.652	-6.874	-0.927	1.00	71.46	B
5851	CA	SER	B1282	25.285	-8.130	-0.803	1.00	70.56	B
5852	CB	SER	B1282	25.774	-8.756	-2.196	1.00	71.93	B
5853	OG	SER	B1282	27.064	-9.608	-2.151	1.00	72.51	B
5854	C	SER	B1282	26.577	-7.826	-0.278	1.00	71.33	B
5855	O	SER	B1282	26.865	-6.966	0.714	1.00	68.41	B
5856	N	ALA	B1283	27.578	-8.420	-1.274	1.00	72.31	B
5857	CA	ALA	B1283	28.499	-9.030	-0.263	1.00	74.23	B
5858	CB	ALA	B1283	27.812	-10.221	0.662	1.00	73.01	B
5859	C	ALA	B1283	29.856	-9.196	-0.345	1.00	74.27	B
5860	O	ALA	B1283	30.373	-10.148	-0.988	1.00	76.21	B
5861	N	ASN	B1284	30.311	-8.554	1.063	1.00	72.80	B
5862	CA	ASN	B1284	31.702	-8.503	1.358	1.00	70.17	B
5863	CB	ASN	B1284	32.153	-8.924	0.011	1.00	69.17	B
5864	CG	ASN	B1284	31.477	-8.015	-1.030	1.00	68.53	B
5865	OD1	ASN	B1284	30.449	-8.320	-1.773	1.00	71.47	B
5866	ND2	ASN	B1284	31.917	-6.811	-0.946	1.00	66.24	B
5867	C	ASN	B1284	32.522	-7.233	1.421	1.00	69.99	B

5868	O	ASN	B1284	33.651	-7.344	1.001	1.00	71.63	B
5869	N	GLN	B1285	32.141	-6.034	1.830	1.00	69.25	B
5870	CA	GLN	B1285	33.226	-5.001	1.658	1.00	69.27	B
5871	CB	GLN	B1285	32.900	-3.756	0.776	1.00	69.92	B
5872	CG	GLN	B1285	33.241	-3.544	-0.793	1.00	68.29	B
5873	CD	GLN	B1285	34.483	-4.247	-1.362	1.00	69.41	B
5874	OE1	GLN	B1285	35.570	-3.647	-1.594	1.00	67.67	B
5875	NE2	GLN	B1285	34.310	-5.499	-1.668	1.00	66.29	B
5876	C	GLN	B1285	33.528	-4.526	3.021	1.00	69.60	B
5877	O	GLN	B1285	32.847	-3.583	3.498	1.00	68.43	B
5878	N	ASP	B1286	34.504	-5.218	3.648	1.00	69.39	B
5879	CA	ASP	B1286	35.271	-4.745	4.792	1.00	69.12	B
5880	CB	ASP	B1286	36.336	-5.802	5.068	1.00	69.48	B
5881	CG	ASP	B1286	37.539	-5.725	4.085	1.00	74.08	B
5882	OD1	ASP	B1286	38.286	-4.685	3.997	1.00	72.38	B
5883	OD2	ASP	B1286	37.757	-6.738	3.365	1.00	83.49	B
5884	C	ASP	B1286	35.879	-3.278	4.668	1.00	67.68	B
5885	O	ASP	B1286	36.698	-2.830	5.459	1.00	67.35	B
5886	N	GLU	B1287	35.452	-2.548	3.651	1.00	67.59	B
5887	CA	GLU	B1287	35.669	-1.085	3.529	1.00	67.02	B
5888	CB	GLU	B1287	35.897	-0.718	2.030	1.00	69.06	B
5889	CG	GLU	B1287	37.289	-1.025	1.436	1.00	65.10	B
5890	CD	GLU	B1287	38.236	0.195	1.539	1.00	69.46	B
5891	OE1	GLU	B1287	37.860	1.340	1.930	1.00	70.53	B
5892	OE2	GLU	B1287	39.415	-0.004	1.237	1.00	71.11	B
5893	C	GLU	B1287	34.413	-0.387	4.031	1.00	65.10	B
5894	O	GLU	B1287	33.294	-0.728	3.629	1.00	64.58	B
5895	N	GLU	B1288	34.558	0.544	4.964	1.00	65.39	B
5896	CA	GLU	B1288	33.359	1.021	5.658	1.00	63.87	B
5897	CB	GLU	B1288	33.455	0.760	7.152	1.00	62.79	B
5898	CG	GLU	B1288	32.284	1.342	8.093	1.00	67.11	B
5899	CD	GLU	B1288	32.684	1.883	9.625	1.00	63.93	B
5900	OE1	GLU	B1288	32.704	1.032	10.546	1.00	54.63	B
5901	OE2	GLU	B1288	32.906	3.149	9.857	1.00	56.11	B
5902	C	GLU	B1288	32.939	2.464	5.198	1.00	65.31	B
5903	O	GLU	B1288	32.602	3.234	6.113	1.00	65.23	B
5904	N	THR	B1289	32.845	2.716	3.807	1.00	62.77	B
5905	CA	THR	B1289	32.285	3.935	3.083	1.00	60.98	B
5906	CB	THR	B1289	32.956	4.278	1.632	1.00	61.43	B
5907	OG1	THR	B1289	32.414	3.450	0.581	1.00	59.96	B
5908	CG2	THR	B1289	34.484	4.369	1.674	1.00	54.59	B
5909	C	THR	B1289	30.844	4.362	2.712	1.00	61.63	B
5910	O	THR	B1289	29.835	4.096	3.379	1.00	64.09	B
5911	N	ASP	B1290	30.748	5.199	1.682	1.00	61.29	B
5912	CA	ASP	B1290	29.441	5.841	1.380	1.00	59.95	B
5913	CB	ASP	B1290	29.595	7.221	0.659	1.00	59.00	B
5914	CG	ASP	B1290	30.179	8.397	1.691	1.00	64.98	B
5915	OD1	ASP	B1290	29.446	9.433	1.969	1.00	52.75	B
5916	OD2	ASP	B1290	31.405	8.236	2.241	1.00	65.74	B
5917	C	ASP	B1290	28.877	4.608	0.677	1.00	58.71	B
5918	O	ASP	B1290	28.298	3.761	1.336	1.00	62.19	B
5919	N	GLN	B1291	29.157	4.303	-0.542	1.00	55.22	B
5920	CA	GLN	B1291	28.723	2.954	-0.997	1.00	52.80	B
5921	CB	GLN	B1291	29.702	2.503	-2.098	1.00	52.14	B
5922	CG	GLN	B1291	30.559	3.698	-2.671	1.00	48.50	B
5923	CD	GLN	B1291	32.007	3.163	-2.981	1.00	60.03	B

5924	OE1	GLN	B1291	32.186	1.967	-3.302	1.00	58.87	B
5925	NE2	GLN	B1291	33.057	4.031	-2.799	1.00	61.18	B
5926	C	GLN	B1291	28.135	1.775	0.057	1.00	52.95	B
5927	O	GLN	B1291	27.086	1.078	-0.178	1.00	53.82	B
5928	N	GLU	B1292	28.752	1.601	1.202	1.00	50.12	B
5929	CA	GLU	B1292	28.265	0.711	2.237	1.00	47.92	B
5930	CB	GLU	B1292	29.481	0.276	2.972	1.00	47.29	B
5931	CG	GLU	B1292	30.438	-0.679	2.128	1.00	45.84	B
5932	CD	GLU	B1292	31.293	-0.074	1.096	1.00	48.41	B
5933	OE1	GLU	B1292	31.616	-0.781	0.109	1.00	45.05	B
5934	OE2	GLU	B1292	31.715	1.118	1.242	1.00	57.23	B
5935	C	GLU	B1292	27.215	1.371	3.195	1.00	49.02	B
5936	O	GLU	B1292	26.488	0.643	3.930	1.00	48.07	B
5937	N	THR	B1293	27.065	2.726	3.125	1.00	47.90	B
5938	CA	THR	B1293	26.214	3.563	4.035	1.00	46.26	B
5939	CB	THR	B1293	26.905	4.888	4.224	1.00	45.49	B
5940	OG1	THR	B1293	28.198	4.579	4.780	1.00	47.05	B
5941	CG2	THR	B1293	26.159	5.871	5.081	1.00	40.33	B
5942	C	THR	B1293	24.780	3.791	3.548	1.00	45.12	B
5943	O	THR	B1293	24.612	4.253	2.467	1.00	45.84	B
5944	N	PHE	B1294	23.850	3.495	4.464	1.00	43.16	B
5945	CA	PHE	B1294	22.440	3.508	4.470	1.00	43.49	B
5946	CB	PHE	B1294	21.924	2.037	4.535	1.00	40.60	B
5947	CG	PHE	B1294	22.731	1.156	3.516	1.00	47.41	B
5948	CD1	PHE	B1294	23.957	0.636	3.840	1.00	41.26	B
5949	CD2	PHE	B1294	22.363	1.098	2.173	1.00	45.04	B
5950	CE1	PHE	B1294	24.730	0.064	2.930	1.00	46.02	B
5951	CE2	PHE	B1294	23.219	0.517	1.244	1.00	46.25	B
5952	CZ	PHE	B1294	24.408	0.039	1.615	1.00	41.13	B
5953	C	PHE	B1294	21.852	4.462	5.563	1.00	46.04	B
5954	O	PHE	B1294	22.353	4.474	6.768	1.00	46.02	B
5955	N	GLN	B1295	20.824	5.234	5.050	1.00	45.82	B
5956	CA	GLN	B1295	20.025	6.177	5.653	1.00	45.74	B
5957	CB	GLN	B1295	19.689	7.216	4.623	1.00	46.67	B
5958	CG	GLN	B1295	18.636	8.396	5.169	1.00	44.91	B
5959	CD	GLN	B1295	19.040	9.783	4.667	1.00	48.38	B
5960	OE1	GLN	B1295	20.282	10.285	4.919	1.00	38.16	B
5961	NE2	GLN	B1295	18.035	10.436	3.834	1.00	42.13	B
5962	C	GLN	B1295	18.739	5.430	5.940	1.00	49.09	B
5963	O	GLN	B1295	17.856	5.224	5.057	1.00	51.41	B
5964	N	LEU	B1296	18.651	5.011	7.190	1.00	47.95	B
5965	CA	LEU	B1296	17.518	4.456	7.795	1.00	47.23	B
5966	CB	LEU	B1296	17.905	4.380	9.237	1.00	46.42	B
5967	CG	LEU	B1296	17.123	3.538	10.133	1.00	44.90	B
5968	CD1	LEU	B1296	17.584	2.201	9.543	1.00	48.45	B
5969	CD2	LEU	B1296	17.459	3.667	11.677	1.00	45.33	B
5970	C	LEU	B1296	16.244	5.297	7.712	1.00	49.43	B
5971	O	LEU	B1296	16.213	6.374	8.294	1.00	52.24	B
5972	N	GLU	B1297	15.146	4.889	7.044	1.00	51.63	B
5973	CA	GLU	B1297	13.960	5.729	7.289	1.00	54.01	B
5974	CB	GLU	B1297	13.413	6.426	6.108	1.00	52.76	B
5975	CG	GLU	B1297	14.341	6.390	4.987	1.00	56.84	B
5976	CD	GLU	B1297	13.886	7.309	4.012	1.00	54.74	B
5977	OE1	GLU	B1297	12.751	7.013	3.438	1.00	54.33	B
5978	OE2	GLU	B1297	14.671	8.280	3.844	1.00	50.71	B
5979	C	GLU	B1297	12.895	5.030	8.041	1.00	56.85	B

5980	O	GLU	B1297	12.936	3.759	8.196	1.00	60.59	B
5981	N	ILE	B1298	11.974	5.829	8.596	1.00	55.95	B
5982	CA	ILE	B1298	10.918	5.258	9.395	1.00	54.31	B
5983	CB	ILE	B1298	11.340	5.330	10.845	1.00	53.39	B
5984	CG2	ILE	B1298	10.248	5.171	11.796	1.00	53.78	B
5985	CG1	ILE	B1298	12.468	4.372	11.149	1.00	52.93	B
5986	CD1	ILE	B1298	13.786	5.163	11.164	1.00	62.50	B
5987	C	ILE	B1298	9.633	6.019	8.925	1.00	55.86	B
5988	O	ILE	B1298	9.707	7.165	8.546	1.00	56.54	B
5989	N	ASP	B1299	8.519	5.337	8.741	1.00	56.21	B
5990	CA	ASP	B1299	7.372	5.970	8.199	1.00	59.62	B
5991	CB	ASP	B1299	6.576	4.937	7.327	1.00	61.15	B
5992	CG	ASP	B1299	6.475	3.618	8.064	1.00	64.57	B
5993	OD1	ASP	B1299	7.498	3.339	8.884	1.00	61.36	B
5994	OD2	ASP	B1299	5.351	3.003	7.960	1.00	64.68	B
5995	C	ASP	B1299	6.666	6.120	9.496	1.00	61.45	B
5996	O	ASP	B1299	6.173	5.028	10.240	1.00	61.29	B
5997	N	ARG	B1300	6.548	7.425	9.788	1.00	61.58	B
5998	CA	ARG	B1300	6.049	7.831	11.086	1.00	62.70	B
5999	CB	ARG	B1300	6.050	9.323	11.266	1.00	62.75	B
6000	CG	ARG	B1300	5.042	10.165	10.577	1.00	63.88	B
6001	CD	ARG	B1300	5.819	11.473	10.315	1.00	70.72	B
6002	NE	ARG	B1300	5.224	12.293	9.252	1.00	69.44	B
6003	CZ	ARG	B1300	5.856	13.143	8.470	1.00	60.52	B
6004	NH1	ARG	B1300	7.142	13.284	8.541	1.00	66.01	B
6005	NH2	ARG	B1300	5.161	13.834	7.611	1.00	63.98	B
6006	C	ARG	B1300	4.741	7.191	11.500	1.00	64.52	B
6007	O	ARG	B1300	4.403	7.307	12.654	1.00	65.00	B
6008	N	ASP	B1301	4.188	6.293	10.659	1.00	66.58	B
6009	CA	ASP	B1301	2.762	5.899	10.674	1.00	67.65	B
6010	CB	ASP	B1301	2.116	6.256	9.298	1.00	68.45	B
6011	CG	ASP	B1301	1.309	7.543	9.301	1.00	62.99	B
6012	OD1	ASP	B1301	1.880	8.617	9.066	1.00	63.76	B
6013	OD2	ASP	B1301	0.063	7.466	9.387	1.00	62.91	B
6014	C	ASP	B1301	2.577	4.378	10.838	1.00	69.76	B
6015	O	ASP	B1301	1.355	3.927	10.856	1.00	68.29	B
6016	N	THR	B1302	3.740	3.622	10.840	1.00	68.85	B
6017	CA	THR	B1302	3.728	2.153	10.945	1.00	66.63	B
6018	CB	THR	B1302	3.038	1.568	9.722	1.00	69.67	B
6019	OG1	THR	B1302	3.372	2.332	8.500	1.00	72.61	B
6020	CG2	THR	B1302	1.442	1.439	9.934	1.00	67.91	B
6021	C	THR	B1302	5.062	1.386	11.107	1.00	65.82	B
6022	O	THR	B1302	5.020	0.135	11.108	1.00	65.31	B
6023	N	LYS	B1303	6.218	2.094	11.203	1.00	64.75	B
6024	CA	LYS	B1303	7.428	1.668	12.019	1.00	62.06	B
6025	CB	LYS	B1303	6.988	0.966	13.289	1.00	60.52	B
6026	CG	LYS	B1303	6.716	1.908	14.489	1.00	56.63	B
6027	CD	LYS	B1303	5.196	2.267	14.503	1.00	55.51	B
6028	CE	LYS	B1303	5.007	3.701	13.942	1.00	58.26	B
6029	NZ	LYS	B1303	6.234	4.100	13.000	1.00	62.52	B
6030	C	LYS	B1303	8.315	0.745	11.304	1.00	63.25	B
6031	O	LYS	B1303	9.501	0.521	11.556	1.00	62.00	B
6032	N	LYS	B1304	7.637	0.102	10.389	1.00	65.99	B
6033	CA	LYS	B1304	8.285	-0.573	9.292	1.00	66.27	B
6034	CB	LYS	B1304	7.246	-0.708	8.214	1.00	66.59	B
6035	CG	LYS	B1304	6.590	-2.034	8.169	1.00	65.83	B

6036	CD	LYS	B1304	7.668	-3.147	8.369	1.00	68.03	B
6037	CE	LYS	B1304	6.917	-4.576	8.385	1.00	64.38	B
6038	NZ	LYS	B1304	6.394	-4.900	9.720	1.00	50.67	B
6039	C	LYS	B1304	9.492	0.296	8.815	1.00	66.51	B
6040	O	LYS	B1304	9.440	1.586	8.717	1.00	62.30	B
6041	N	CYS	B1305	10.611	-0.437	8.676	1.00	67.26	B
6042	CA	CYS	B1305	11.859	0.173	8.202	1.00	65.85	B
6043	CB	CYS	B1305	13.027	-0.616	8.635	1.00	63.20	B
6044	SG	CYS	B1305	14.485	0.134	8.117	1.00	68.55	B
6045	C	CYS	B1305	11.829	0.266	6.661	1.00	65.64	B
6046	O	CYS	B1305	10.849	-0.211	5.972	1.00	65.20	B
6047	N	ALA	B1306	12.873	0.972	6.184	1.00	64.19	B
6048	CA	ALA	B1306	13.362	1.022	4.818	1.00	61.03	B
6049	CB	ALA	B1306	12.415	1.829	3.956	1.00	58.21	B
6050	C	ALA	B1306	14.831	1.577	4.776	1.00	60.20	B
6051	O	ALA	B1306	15.064	2.730	5.142	1.00	60.56	B
6052	N	PHE	B1307	15.798	0.780	4.319	1.00	60.07	B
6053	CA	PHE	B1307	17.130	1.317	3.932	1.00	61.29	B
6054	CB	PHE	B1307	18.195	0.245	3.992	1.00	61.40	B
6055	CG	PHE	B1307	18.092	-0.659	5.213	1.00	63.89	B
6056	CD1	PHE	B1307	17.005	-1.568	5.345	1.00	54.51	B
6057	CD2	PHE	B1307	19.071	-0.576	6.243	1.00	58.95	B
6058	CE1	PHE	B1307	16.900	-2.291	6.463	1.00	56.65	B
6059	CE2	PHE	B1307	18.979	-1.396	7.414	1.00	60.64	B
6060	CZ	PHE	B1307	17.942	-2.220	7.546	1.00	59.31	B
6061	C	PHE	B1307	17.258	2.029	2.520	1.00	61.72	B
6062	O	PHE	B1307	16.811	1.524	1.515	1.00	62.99	B
6063	N	ARG	B1308	17.909	3.191	2.534	1.00	59.31	B
6064	CA	ARG	B1308	18.153	3.993	1.439	1.00	57.15	B
6065	CB	ARG	B1308	17.801	5.423	1.846	1.00	58.46	B
6066	CG	ARG	B1308	17.841	6.337	0.642	1.00	55.44	B
6067	CD	ARG	B1308	16.759	7.356	0.726	1.00	55.96	B
6068	NE	ARG	B1308	16.737	8.111	-0.525	1.00	53.61	B
6069	CZ	ARG	B1308	15.692	8.672	-1.038	1.00	54.08	B
6070	NH1	ARG	B1308	14.525	8.689	-0.443	1.00	57.59	B
6071	NH2	ARG	B1308	15.844	9.277	-2.138	1.00	61.30	B
6072	C	ARG	B1308	19.625	4.090	1.108	1.00	56.45	B
6073	O	ARG	B1308	20.439	4.390	1.985	1.00	57.59	B
6074	N	THR	B1309	19.978	3.982	-0.174	1.00	53.61	B
6075	CA	THR	B1309	21.424	3.976	-0.540	1.00	49.79	B
6076	CB	THR	B1309	21.718	3.070	-1.711	1.00	46.51	B
6077	OG1	THR	B1309	21.169	3.707	-2.948	1.00	55.46	B
6078	CG2	THR	B1309	21.076	1.770	-1.491	1.00	26.74	B
6079	C	THR	B1309	21.678	5.422	-0.891	1.00	52.22	B
6080	O	THR	B1309	20.715	6.175	-1.100	1.00	50.44	B
6081	N	HIS	B1310	22.968	5.769	-0.808	1.00	55.09	B
6082	CA	HIS	B1310	23.663	6.987	-1.332	1.00	57.71	B
6083	CB	HIS	B1310	25.182	6.761	-1.192	1.00	56.85	B
6084	CG	HIS	B1310	25.673	5.633	-2.051	1.00	55.67	B
6085	CD2	HIS	B1310	25.037	4.545	-2.519	1.00	55.09	B
6086	ND1	HIS	B1310	26.938	5.581	-2.584	1.00	51.62	B
6087	CE1	HIS	B1310	27.051	4.518	-3.361	1.00	42.33	B
6088	NE2	HIS	B1310	25.901	3.899	-3.369	1.00	52.27	B
6089	C	HIS	B1310	23.400	7.386	-2.821	1.00	58.84	B
6090	O	HIS	B1310	23.219	8.547	-3.100	1.00	61.23	B
6091	N	THR	B1311	23.362	6.435	-3.725	1.00	58.38	B

6092	CA	THR	B1311	22.934	6.721	-5.058	1.00	59.83	B
6093	CB	THR	B1311	23.411	5.606	-6.204	1.00	60.47	B
6094	OG1	THR	B1311	22.363	4.687	-6.539	1.00	68.05	B
6095	CG2	THR	B1311	24.757	4.810	-5.803	1.00	59.16	B
6096	C	THR	B1311	21.450	7.114	-5.102	1.00	57.96	B
6097	O	THR	B1311	20.938	7.436	-6.209	1.00	56.32	B
6098	N	GLY	B1312	20.777	7.108	-3.919	1.00	56.46	B
6099	CA	GLY	B1312	19.358	7.627	-3.810	1.00	53.19	B
6100	C	GLY	B1312	18.233	6.582	-3.909	1.00	54.21	B
6101	O	GLY	B1312	17.049	6.926	-3.902	1.00	51.84	B
6102	N	LYS	B1313	18.591	5.284	-3.923	1.00	55.29	B
6103	CA	LYS	B1313	17.671	4.277	-4.412	1.00	56.06	B
6104	CB	LYS	B1313	18.277	3.389	-5.499	1.00	58.35	B
6105	CG	LYS	B1313	18.390	3.915	-6.980	1.00	50.73	B
6106	CD	LYS	B1313	17.141	4.415	-7.500	1.00	51.74	B
6107	CE	LYS	B1313	17.410	5.941	-8.232	1.00	62.24	B
6108	NZ	LYS	B1313	18.824	6.311	-8.776	1.00	56.63	B
6109	C	LYS	B1313	17.455	3.412	-3.329	1.00	58.67	B
6110	O	LYS	B1313	18.222	3.439	-2.363	1.00	61.02	B
6111	N	TYR	B1314	16.412	2.594	-3.421	1.00	59.76	B
6112	CA	TYR	B1314	16.066	1.871	-2.158	1.00	59.62	B
6113	CB	TYR	B1314	14.621	2.223	-1.802	1.00	60.86	B
6114	CG	TYR	B1314	14.272	3.585	-1.261	1.00	60.10	B
6115	CD1	TYR	B1314	13.665	4.543	-2.072	1.00	68.28	B
6116	CE1	TYR	B1314	13.248	5.793	-1.539	1.00	70.74	B
6117	CD2	TYR	B1314	14.456	3.875	0.060	1.00	62.18	B
6118	CE2	TYR	B1314	14.073	5.102	0.614	1.00	65.03	B
6119	CZ	TYR	B1314	13.453	6.050	-0.173	1.00	64.15	B
6120	OH	TYR	B1314	13.089	7.252	0.372	1.00	58.23	B
6121	C	TYR	B1314	16.054	0.390	-2.244	1.00	58.39	B
6122	O	TYR	B1314	15.649	-0.165	-3.246	1.00	60.02	B
6123	N	TRP	B1315	16.386	-0.266	-1.161	1.00	57.78	B
6124	CA	TRP	B1315	16.130	-1.743	-0.963	1.00	56.84	B
6125	CB	TRP	B1315	16.222	-2.097	0.566	1.00	53.73	B
6126	CG	TRP	B1315	17.592	-1.807	1.055	1.00	50.83	B
6127	CD2	TRP	B1315	18.430	-2.589	1.930	1.00	39.53	B
6128	CE2	TRP	B1315	19.717	-1.900	2.028	1.00	46.80	B
6129	CE3	TRP	B1315	18.242	-3.731	2.643	1.00	46.39	B
6130	CD1	TRP	B1315	18.372	-0.695	0.692	1.00	51.40	B
6131	NE1	TRP	B1315	19.657	-0.766	1.236	1.00	50.92	B
6132	CZ2	TRP	B1315	20.765	-2.332	2.843	1.00	51.30	B
6133	CZ3	TRP	B1315	19.383	-4.222	3.484	1.00	55.04	B
6134	CH2	TRP	B1315	20.608	-3.510	3.558	1.00	52.28	B
6135	C	TRP	B1315	14.759	-2.242	-1.572	1.00	56.61	B
6136	O	TRP	B1315	13.727	-1.755	-1.202	1.00	57.26	B
6137	N	THR	B1316	14.735	-3.199	-2.469	1.00	56.17	B
6138	CA	THR	B1316	13.479	-3.755	-2.848	1.00	56.93	B
6139	CB	THR	B1316	12.829	-3.007	-4.219	1.00	58.26	B
6140	OG1	THR	B1316	11.513	-2.458	-3.980	1.00	49.29	B
6141	CG2	THR	B1316	12.835	-3.933	-5.527	1.00	57.58	B
6142	C	THR	B1316	13.731	-5.287	-2.874	1.00	60.25	B
6143	O	THR	B1316	14.929	-5.852	-3.128	1.00	61.25	B
6144	N	LEU	B1317	12.638	-5.998	-2.582	1.00	59.97	B
6145	CA	LEU	B1317	12.715	-7.432	-2.325	1.00	59.15	B
6146	CB	LEU	B1317	11.549	-7.718	-1.442	1.00	58.33	B
6147	CG	LEU	B1317	11.073	-8.918	-0.673	1.00	55.02	B

6148	CD1	LEU	B1317	10.132	-9.320	-1.695	1.00	56.53	B
6149	CD2	LEU	B1317	12.135	-10.022	-0.117	1.00	32.65	B
6150	C	LEU	B1317	12.454	-7.965	-3.636	1.00	60.10	B
6151	O	LEU	B1317	11.471	-7.581	-4.330	1.00	62.00	B
6152	N	THR	B1318	13.354	-8.794	-4.086	1.00	60.87	B
6153	CA	THR	B1318	13.051	-9.314	-5.408	1.00	61.41	B
6154	CB	THR	B1318	14.264	-9.514	-6.241	1.00	59.83	B
6155	OG1	THR	B1318	15.082	-10.476	-5.588	1.00	62.57	B
6156	CG2	THR	B1318	15.054	-8.215	-6.591	1.00	53.60	B
6157	C	THR	B1318	12.240	-10.634	-5.249	1.00	64.33	B
6158	O	THR	B1318	11.177	-10.611	-4.519	1.00	65.34	B
6159	N	ALA	B1319	12.735	-11.721	-5.880	1.00	64.73	B
6160	CA	ALA	B1319	12.079	-13.054	-6.111	1.00	64.72	B
6161	CB	ALA	B1319	11.622	-13.311	-7.620	1.00	63.67	B
6162	C	ALA	B1319	13.161	-14.062	-5.798	1.00	66.25	B
6163	O	ALA	B1319	12.885	-14.891	-4.949	1.00	65.48	B
6164	N	THR	B1320	14.370	-13.976	-6.457	1.00	65.75	B
6165	CA	THR	B1320	15.594	-14.659	-5.995	1.00	68.30	B
6166	CB	THR	B1320	16.950	-13.965	-6.368	1.00	68.57	B
6167	OG1	THR	B1320	16.785	-13.129	-7.489	1.00	76.61	B
6168	CG2	THR	B1320	18.067	-15.026	-6.713	1.00	69.24	B
6169	C	THR	B1320	15.726	-14.687	-4.455	1.00	67.88	B
6170	O	THR	B1320	16.876	-14.814	-3.881	1.00	69.95	B
6171	N	GLY	B1321	14.607	-14.523	-3.774	1.00	65.50	B
6172	CA	GLY	B1321	14.653	-13.887	-2.472	1.00	63.65	B
6173	C	GLY	B1321	15.746	-12.890	-2.217	1.00	60.50	B
6174	O	GLY	B1321	16.169	-12.771	-1.050	1.00	62.39	B
6175	N	GLY	B1322	16.182	-12.160	-3.285	1.00	59.07	B
6176	CA	GLY	B1322	17.477	-11.389	-3.310	1.00	50.95	B
6177	C	GLY	B1322	16.918	-10.053	-2.994	1.00	49.26	B
6178	O	GLY	B1322	15.661	-9.797	-3.103	1.00	47.92	B
6179	N	VAL	B1323	17.800	-9.196	-2.565	1.00	48.32	B
6180	CA	VAL	B1323	17.380	-7.865	-2.324	1.00	49.35	B
6181	CB	VAL	B1323	17.032	-7.580	-0.648	1.00	49.82	B
6182	CG1	VAL	B1323	16.611	-6.024	-0.434	1.00	46.14	B
6183	CG2	VAL	B1323	15.933	-8.664	0.023	1.00	39.69	B
6184	C	VAL	B1323	18.400	-6.869	-2.920	1.00	51.45	B
6185	O	VAL	B1323	19.647	-7.022	-2.852	1.00	49.90	B
6186	N	GLN	B1324	17.889	-5.769	-3.400	1.00	53.71	B
6187	CA	GLN	B1324	18.634	-5.135	-4.439	1.00	58.47	B
6188	CB	GLN	B1324	18.352	-5.816	-5.862	1.00	59.38	B
6189	CG	GLN	B1324	18.963	-7.325	-6.077	1.00	60.37	B
6190	CD	GLN	B1324	18.617	-7.998	-7.525	1.00	64.75	B
6191	OE1	GLN	B1324	18.748	-9.219	-7.647	1.00	69.06	B
6192	NE2	GLN	B1324	18.188	-7.204	-8.574	1.00	56.78	B
6193	C	GLN	B1324	18.153	-3.722	-4.337	1.00	57.91	B
6194	O	GLN	B1324	17.014	-3.439	-3.797	1.00	60.51	B
6195	N	SER	B1325	18.953	-2.779	-4.820	1.00	55.94	B
6196	CA	SER	B1325	18.582	-1.444	-4.355	1.00	54.92	B
6197	CB	SER	B1325	19.734	-0.834	-3.635	1.00	52.57	B
6198	OG	SER	B1325	20.516	-0.134	-4.457	1.00	45.46	B
6199	C	SER	B1325	18.009	-0.607	-5.434	1.00	55.72	B
6200	O	SER	B1325	18.707	0.233	-6.032	1.00	56.08	B
6201	N	THR	B1326	16.740	-0.824	-5.698	1.00	56.01	B
6202	CA	THR	B1326	16.234	-0.295	-6.911	1.00	58.59	B
6203	CB	THR	B1326	15.908	-1.416	-7.673	1.00	57.91	B

6204	OG1	THR	B1326	17.087	-1.582	-8.480	1.00	63.81	B
6205	CG2	THR	B1326	14.519	-1.239	-8.507	1.00	58.53	B
6206	C	THR	B1326	15.144	0.725	-6.952	1.00	60.15	B
6207	O	THR	B1326	15.232	1.758	-7.657	1.00	62.95	B
6208	N	ALA	B1327	14.055	0.393	-6.317	1.00	62.23	B
6209	CA	ALA	B1327	13.028	1.367	-6.075	1.00	64.94	B
6210	CB	ALA	B1327	12.194	1.003	-4.722	1.00	64.67	B
6211	C	ALA	B1327	13.612	2.785	-5.961	1.00	64.80	B
6212	O	ALA	B1327	14.447	3.095	-5.118	1.00	65.82	B
6213	N	SER	B1328	13.146	3.571	-6.868	1.00	65.40	B
6214	CA	SER	B1328	13.283	4.963	-6.948	1.00	69.15	B
6215	CB	SER	B1328	13.036	5.312	-8.434	1.00	69.00	B
6216	OG	SER	B1328	13.732	4.342	-9.312	1.00	79.01	B
6217	C	SER	B1328	12.224	5.679	-6.049	1.00	69.31	B
6218	O	SER	B1328	12.528	6.732	-5.443	1.00	70.51	B
6219	N	SER	B1329	10.967	5.165	-6.027	1.00	69.53	B
6220	CA	SER	B1329	9.948	5.547	-5.015	1.00	67.45	B
6221	CB	SER	B1329	8.572	5.833	-5.630	1.00	68.11	B
6222	OG	SER	B1329	7.963	6.925	-4.919	1.00	64.39	B
6223	C	SER	B1329	9.850	4.643	-3.730	1.00	66.29	B
6224	O	SER	B1329	10.541	3.708	-3.546	1.00	66.02	B
6225	N	LYS	B1330	9.026	5.059	-2.819	1.00	65.44	B
6226	CA	LYS	B1330	8.741	4.423	-1.563	1.00	65.66	B
6227	CB	LYS	B1330	8.179	5.569	-0.712	1.00	66.32	B
6228	CG	LYS	B1330	8.609	7.061	-1.427	1.00	67.86	B
6229	CD	LYS	B1330	8.126	8.342	-0.690	1.00	67.00	B
6230	CE	LYS	B1330	7.745	8.078	0.801	1.00	63.76	B
6231	NZ	LYS	B1330	6.276	8.412	1.169	1.00	63.23	B
6232	C	LYS	B1330	7.740	3.232	-1.741	1.00	65.41	B
6233	O	LYS	B1330	6.771	3.021	-0.956	1.00	64.30	B
6234	N	ASN	B1331	7.943	2.437	-2.774	1.00	64.27	B
6235	CA	ASN	B1331	7.248	1.130	-2.722	1.00	65.65	B
6236	CB	ASN	B1331	7.570	0.156	-3.974	1.00	65.80	B
6237	CG	ASN	B1331	7.476	-1.357	-3.606	1.00	63.16	B
6238	OD1	ASN	B1331	8.273	-2.169	-4.005	1.00	57.47	B
6239	ND2	ASN	B1331	6.524	-1.680	-2.786	1.00	64.91	B
6240	C	ASN	B1331	7.278	0.416	-1.284	1.00	64.30	B
6241	O	ASN	B1331	8.309	0.258	-0.625	1.00	62.23	B
6242	N	ALA	B1332	6.097	-0.049	-0.904	1.00	63.96	B
6243	CA	ALA	B1332	5.892	-0.814	0.262	1.00	65.17	B
6244	CB	ALA	B1332	4.451	-0.774	0.663	1.00	66.91	B
6245	C	ALA	B1332	6.378	-2.236	0.020	1.00	65.70	B
6246	O	ALA	B1332	6.073	-3.170	0.779	1.00	65.59	B
6247	N	SER	B1333	7.281	-2.331	-0.957	1.00	65.47	B
6248	CA	SER	B1333	8.079	-3.532	-1.254	1.00	65.65	B
6249	CB	SER	B1333	8.324	-3.504	-2.760	1.00	65.16	B
6250	OG	SER	B1333	8.202	-4.795	-3.330	1.00	71.97	B
6251	C	SER	B1333	9.409	-3.430	-0.534	1.00	63.68	B
6252	O	SER	B1333	10.250	-4.432	-0.440	1.00	60.52	B
6253	N	CYS	B1334	9.608	-2.180	-0.068	1.00	62.46	B
6254	CA	CYS	B1334	10.952	-1.785	0.365	1.00	62.56	B
6255	CB	CYS	B1334	11.339	-0.479	-0.251	1.00	61.17	B
6256	SG	CYS	B1334	10.595	-0.216	-1.812	1.00	62.57	B
6257	C	CYS	B1334	11.084	-1.670	1.899	1.00	62.62	B
6258	O	CYS	B1334	12.161	-1.224	2.395	1.00	60.98	B
6259	N	TYR	B1335	9.989	-2.088	2.580	1.00	61.56	B

6260	CA	TYR	B1335	9.715	-1.854	3.972	1.00	61.58	B
6261	CB	TYR	B1335	8.296	-1.364	4.075	1.00	62.45	B
6262	CG	TYR	B1335	8.156	0.125	3.947	1.00	67.38	B
6263	CD1	TYR	B1335	7.882	0.732	2.714	1.00	66.79	B
6264	CE1	TYR	B1335	7.685	2.070	2.624	1.00	63.09	B
6265	CD2	TYR	B1335	8.224	0.960	5.084	1.00	69.90	B
6266	CE2	TYR	B1335	8.070	2.363	4.969	1.00	66.60	B
6267	CZ	TYR	B1335	7.826	2.887	3.746	1.00	66.48	B
6268	OH	TYR	B1335	7.648	4.283	3.672	1.00	72.75	B
6269	C	TYR	B1335	9.945	-3.108	4.830	1.00	60.91	B
6270	O	TYR	B1335	9.077	-3.969	5.035	1.00	59.64	B
6271	N	PHE	B1336	11.138	-3.186	5.365	1.00	62.32	B
6272	CA	PHE	B1336	11.545	-4.284	6.202	1.00	63.37	B
6273	CB	PHE	B1336	13.021	-4.484	5.980	1.00	64.69	B
6274	CG	PHE	B1336	13.303	-5.173	4.639	1.00	68.16	B
6275	CD1	PHE	B1336	14.462	-5.858	4.414	1.00	69.57	B
6276	CD2	PHE	B1336	12.295	-5.211	3.616	1.00	73.01	B
6277	CE1	PHE	B1336	14.661	-6.520	3.194	1.00	70.99	B
6278	CE2	PHE	B1336	12.442	-5.943	2.382	1.00	68.68	B
6279	CZ	PHE	B1336	13.625	-6.574	2.160	1.00	69.34	B
6280	C	PHE	B1336	11.127	-4.034	7.627	1.00	64.54	B
6281	O	PHE	B1336	11.450	-3.032	8.311	1.00	64.17	B
6282	N	ASP	B1337	10.309	-4.940	8.094	1.00	64.71	B
6283	CA	ASP	B1337	10.291	-5.065	9.585	1.00	64.08	B
6284	CB	ASP	B1337	9.868	-6.461	9.935	1.00	64.52	B
6285	CG	ASP	B1337	8.954	-6.402	10.883	1.00	67.54	B
6286	OD1	ASP	B1337	8.836	-7.457	11.647	1.00	71.17	B
6287	OD2	ASP	B1337	8.471	-5.167	10.856	1.00	61.75	B
6288	C	ASP	B1337	11.639	-4.958	10.300	1.00	60.74	B
6289	O	ASP	B1337	12.470	-5.869	10.113	1.00	56.39	B
6290	N	ILE	B1338	11.820	-3.995	11.199	1.00	59.42	B
6291	CA	ILE	B1338	12.913	-4.299	12.192	1.00	60.22	B
6292	CB	ILE	B1338	13.885	-3.163	12.459	1.00	58.76	B
6293	CG2	ILE	B1338	14.879	-3.759	13.212	1.00	58.20	B
6294	CG1	ILE	B1338	14.628	-2.712	11.179	1.00	58.40	B
6295	CD1	ILE	B1338	15.136	-1.195	11.182	1.00	57.91	B
6296	C	ILE	B1338	12.498	-5.012	13.527	1.00	61.22	B
6297	O	ILE	B1338	11.467	-4.668	14.141	1.00	61.21	B
6298	N	GLU	B1339	13.227	-6.057	13.956	1.00	61.41	B
6299	CA	GLU	B1339	13.063	-6.493	15.415	1.00	59.86	B
6300	CB	GLU	B1339	12.677	-7.964	15.657	1.00	58.57	B
6301	CG	GLU	B1339	13.417	-8.693	16.932	1.00	59.01	B
6302	CD	GLU	B1339	14.260	-10.010	16.620	1.00	58.34	B
6303	OE1	GLU	B1339	13.736	-10.888	15.901	1.00	59.31	B
6304	OE2	GLU	B1339	15.434	-10.134	17.051	1.00	57.05	B
6305	C	GLU	B1339	14.342	-6.117	16.148	1.00	60.00	B
6306	O	GLU	B1339	15.431	-6.312	15.594	1.00	59.83	B
6307	N	TRP	B1340	14.187	-5.583	17.381	1.00	61.54	B
6308	CA	TRP	B1340	15.214	-4.920	18.177	1.00	60.26	B
6309	CB	TRP	B1340	14.519	-3.817	18.954	1.00	58.16	B
6310	CG	TRP	B1340	14.188	-2.662	17.948	1.00	56.03	B
6311	CD2	TRP	B1340	15.099	-1.945	17.095	1.00	52.75	B
6312	CE2	TRP	B1340	14.340	-1.044	16.312	1.00	56.59	B
6313	CE3	TRP	B1340	16.499	-1.868	17.013	1.00	56.23	B
6314	CD1	TRP	B1340	12.925	-2.240	17.563	1.00	56.95	B
6315	NE1	TRP	B1340	13.011	-1.239	16.604	1.00	50.79	B

6316	CZ2	TRP	B1340	14.970	-0.085	15.377	1.00	60.02	B
6317	CZ3	TRP	B1340	17.136	-0.906	16.125	1.00	52.28	B
6318	CH2	TRP	B1340	16.359	-0.054	15.314	1.00	56.05	B
6319	C	TRP	B1340	15.826	-5.956	19.014	1.00	61.27	B
6320	O	TRP	B1340	15.278	-6.284	20.024	1.00	61.18	B
6321	N	ARG	B1341	16.909	-6.571	18.517	1.00	63.30	B
6322	CA	ARG	B1341	17.341	-7.940	19.055	1.00	63.38	B
6323	CB	ARG	B1341	17.455	-9.043	17.915	1.00	64.35	B
6324	CG	ARG	B1341	17.546	-10.589	18.270	1.00	68.12	B
6325	CD	ARG	B1341	18.626	-11.047	19.473	1.00	75.04	B
6326	NE	ARG	B1341	19.461	-12.228	19.199	1.00	69.85	B
6327	CZ	ARG	B1341	20.741	-12.327	19.569	1.00	70.89	B
6328	NH1	ARG	B1341	21.285	-11.324	20.281	1.00	65.96	B
6329	NH2	ARG	B1341	21.473	-13.444	19.256	1.00	62.21	B
6330	C	ARG	B1341	18.622	-7.540	19.827	1.00	61.16	B
6331	O	ARG	B1341	19.472	-8.269	20.203	1.00	56.86	B
6332	N	ASP	B1342	18.617	-6.260	20.080	1.00	62.48	B
6333	CA	ASP	B1342	19.538	-5.551	21.035	1.00	61.62	B
6334	CB	ASP	B1342	19.153	-5.826	22.423	1.00	61.06	B
6335	CG	ASP	B1342	17.816	-5.424	22.623	1.00	64.82	B
6336	OD1	ASP	B1342	17.498	-4.388	21.951	1.00	64.19	B
6337	OD2	ASP	B1342	17.089	-6.133	23.392	1.00	68.92	B
6338	C	ASP	B1342	20.984	-5.783	20.868	1.00	59.96	B
6339	O	ASP	B1342	21.460	-6.749	21.485	1.00	59.52	B
6340	N	ARG	B1343	21.622	-4.973	19.998	1.00	55.88	B
6341	CA	ARG	B1343	23.001	-5.222	19.594	1.00	54.99	B
6342	CB	ARG	B1343	23.769	-5.671	20.822	1.00	55.95	B
6343	CG	ARG	B1343	25.225	-5.916	20.750	1.00	56.80	B
6344	CD	ARG	B1343	25.361	-7.082	21.772	1.00	65.03	B
6345	NE	ARG	B1343	25.314	-6.764	23.197	1.00	59.82	B
6346	CZ	ARG	B1343	26.245	-6.043	23.726	1.00	61.56	B
6347	NH1	ARG	B1343	27.202	-5.571	22.969	1.00	66.89	B
6348	NH2	ARG	B1343	26.272	-5.834	24.991	1.00	66.47	B
6349	C	ARG	B1343	23.243	-6.151	18.439	1.00	54.47	B
6350	O	ARG	B1343	24.370	-6.580	18.180	1.00	56.15	B
6351	N	ARG	B1344	22.184	-6.512	17.756	1.00	53.53	B
6352	CA	ARG	B1344	22.224	-7.300	16.552	1.00	52.75	B
6353	CB	ARG	B1344	22.961	-8.652	16.661	1.00	52.87	B
6354	CG	ARG	B1344	24.518	-8.518	16.251	1.00	53.39	B
6355	CD	ARG	B1344	25.638	-8.893	17.381	1.00	55.76	B
6356	NE	ARG	B1344	27.020	-8.390	17.094	1.00	54.08	B
6357	CZ	ARG	B1344	27.943	-8.150	18.037	1.00	50.24	B
6358	NH1	ARG	B1344	29.113	-7.570	17.751	1.00	30.40	B
6359	NH2	ARG	B1344	27.701	-8.476	19.314	1.00	58.72	B
6360	C	ARG	B1344	20.812	-7.380	16.474	1.00	52.45	B
6361	O	ARG	B1344	20.104	-7.160	17.512	1.00	55.12	B
6362	N	ILE	B1345	20.362	-7.537	15.248	1.00	53.22	B
6363	CA	ILE	B1345	19.056	-7.037	14.789	1.00	52.19	B
6364	CB	ILE	B1345	19.254	-5.573	14.411	1.00	53.37	B
6365	CG2	ILE	B1345	18.018	-5.026	13.626	1.00	54.05	B
6366	CG1	ILE	B1345	19.076	-4.672	15.656	1.00	55.15	B
6367	CD1	ILE	B1345	20.265	-3.784	16.406	1.00	48.51	B
6368	C	ILE	B1345	18.506	-7.863	13.560	1.00	52.77	B
6369	O	ILE	B1345	19.241	-8.605	12.860	1.00	49.66	B
6370	N	THR	B1346	17.214	-7.797	13.274	1.00	53.63	B
6371	CA	THR	B1346	16.761	-8.918	12.405	1.00	55.23	B

6372	CB	THR	B1346	15.876	-10.114	13.126	1.00	57.65	B
6373	OG1	THR	B1346	16.437	-10.580	14.401	1.00	57.45	B
6374	CG2	THR	B1346	15.751	-11.271	12.172	1.00	55.04	B
6375	C	THR	B1346	15.856	-8.335	11.471	1.00	55.72	B
6376	O	THR	B1346	14.718	-7.745	11.856	1.00	55.09	B
6377	N	LEU	B1347	16.333	-8.461	10.237	1.00	55.36	B
6378	CA	LEU	B1347	15.515	-7.878	9.238	1.00	54.29	B
6379	CB	LEU	B1347	16.342	-7.183	8.218	1.00	55.56	B
6380	CG	LEU	B1347	17.099	-5.898	8.247	1.00	56.22	B
6381	CD1	LEU	B1347	17.993	-5.910	9.523	1.00	51.61	B
6382	CD2	LEU	B1347	17.929	-5.948	6.799	1.00	52.01	B
6383	C	LEU	B1347	14.593	-9.022	8.697	1.00	52.51	B
6384	O	LEU	B1347	15.059	-10.115	8.731	1.00	53.13	B
6385	N	ARG	B1348	13.413	-8.681	8.183	1.00	48.76	B
6386	CA	ARG	B1348	12.261	-9.417	8.079	1.00	51.51	B
6387	CB	ARG	B1348	11.570	-9.674	9.498	1.00	55.09	B
6388	CG	ARG	B1348	11.913	-11.228	10.343	1.00	54.89	B
6389	CD	ARG	B1348	10.619	-12.100	10.849	1.00	49.11	B
6390	NE	ARG	B1348	9.520	-11.080	11.107	1.00	64.61	B
6391	CZ	ARG	B1348	8.780	-10.781	12.232	1.00	60.68	B
6392	NH1	ARG	B1348	8.891	-11.468	13.352	1.00	65.67	B
6393	NH2	ARG	B1348	7.889	-9.748	12.258	1.00	55.16	B
6394	C	ARG	B1348	11.291	-8.792	6.960	1.00	53.82	B
6395	O	ARG	B1348	10.413	-7.777	7.056	1.00	51.71	B
6396	N	ALA	B1349	11.529	-9.440	5.831	1.00	54.47	B
6397	CA	ALA	B1349	11.299	-8.900	4.552	1.00	55.85	B
6398	CB	ALA	B1349	11.976	-9.763	3.583	1.00	54.99	B
6399	C	ALA	B1349	9.811	-8.858	4.381	1.00	57.33	B
6400	O	ALA	B1349	9.122	-9.186	5.301	1.00	56.70	B
6401	N	SER	B1350	9.368	-8.337	3.243	1.00	60.28	B
6402	CA	SER	B1350	8.076	-8.609	2.564	1.00	61.18	B
6403	CB	SER	B1350	8.037	-7.843	1.150	1.00	62.71	B
6404	OG	SER	B1350	8.564	-6.423	0.971	1.00	59.40	B
6405	C	SER	B1350	7.779	-10.194	2.361	1.00	62.39	B
6406	O	SER	B1350	6.632	-10.643	1.993	1.00	64.67	B
6407	N	ASN	B1351	8.791	-11.016	2.624	1.00	60.61	B
6408	CA	ASN	B1351	8.765	-12.522	2.482	1.00	59.12	B
6409	CB	ASN	B1351	9.716	-12.871	1.321	1.00	58.24	B
6410	CG	ASN	B1351	11.273	-12.628	1.682	1.00	61.23	B
6411	OD1	ASN	B1351	11.687	-11.476	1.961	1.00	61.99	B
6412	ND2	ASN	B1351	12.141	-13.709	1.590	1.00	61.26	B
6413	C	ASN	B1351	9.074	-13.571	3.762	1.00	57.41	B
6414	O	ASN	B1351	9.458	-14.741	3.520	1.00	55.30	B
6415	N	GLY	B1352	8.791	-13.184	5.024	1.00	56.17	B
6416	CA	GLY	B1352	9.381	-13.768	6.274	1.00	53.52	B
6417	C	GLY	B1352	10.911	-13.752	6.392	1.00	52.25	B
6418	O	GLY	B1352	11.666	-12.750	6.477	1.00	48.19	B
6419	N	LYS	B1353	11.366	-14.982	6.448	1.00	54.18	B
6420	CA	LYS	B1353	12.720	-15.360	6.677	1.00	54.61	B
6421	CB	LYS	B1353	13.192	-16.353	5.599	1.00	54.63	B
6422	CG	LYS	B1353	12.791	-16.150	4.309	1.00	51.56	B
6423	CD	LYS	B1353	12.410	-17.486	3.732	1.00	55.63	B
6424	CE	LYS	B1353	11.204	-17.299	2.606	1.00	56.61	B
6425	NZ	LYS	B1353	9.616	-17.055	3.045	1.00	49.42	B
6426	C	LYS	B1353	13.721	-14.206	6.840	1.00	57.90	B
6427	O	LYS	B1353	13.548	-12.989	6.389	1.00	53.36	B

6428	N	PHE	B1354	14.774	-14.640	7.565	1.00	60.54	B
6429	CA	PHE	B1354	15.839	-13.729	8.096	1.00	62.38	B
6430	CB	PHE	B1354	16.428	-14.241	9.402	1.00	61.68	B
6431	CG	PHE	B1354	15.390	-14.689	10.399	1.00	62.33	B
6432	CD1	PHE	B1354	14.453	-13.820	10.903	1.00	67.23	B
6433	CD2	PHE	B1354	15.372	-15.982	10.852	1.00	57.79	B
6434	CE1	PHE	B1354	13.495	-14.279	11.797	1.00	68.78	B
6435	CE2	PHE	B1354	14.479	-16.407	11.701	1.00	52.22	B
6436	CZ	PHE	B1354	13.526	-15.569	12.177	1.00	63.72	B
6437	C	PHE	B1354	16.904	-13.345	7.091	1.00	63.46	B
6438	O	PHE	B1354	17.840	-14.029	6.696	1.00	63.89	B
6439	N	VAL	B1355	16.702	-12.216	6.557	1.00	65.02	B
6440	CA	VAL	B1355	17.783	-11.646	5.848	1.00	64.85	B
6441	CB	VAL	B1355	17.453	-10.088	5.882	1.00	66.01	B
6442	CG1	VAL	B1355	18.601	-9.236	5.355	1.00	62.57	B
6443	CG2	VAL	B1355	15.844	-9.822	5.352	1.00	54.98	B
6444	C	VAL	B1355	19.127	-12.084	6.522	1.00	65.47	B
6445	O	VAL	B1355	19.471	-11.525	7.578	1.00	63.12	B
6446	N	THR	B1356	19.812	-13.132	5.927	1.00	66.86	B
6447	CA	THR	B1356	21.345	-13.459	6.100	1.00	66.83	B
6448	CB	THR	B1356	21.612	-15.001	6.295	1.00	67.30	B
6449	OG1	THR	B1356	23.011	-15.323	5.958	1.00	64.76	B
6450	CG2	THR	B1356	20.651	-15.747	5.537	1.00	60.99	B
6451	C	THR	B1356	22.555	-12.880	5.149	1.00	68.10	B
6452	O	THR	B1356	22.676	-11.656	4.975	1.00	68.42	B
6453	N	SER	B1357	23.443	-13.742	4.585	1.00	67.23	B
6454	CA	SER	B1357	24.636	-13.291	3.855	1.00	67.37	B
6455	CB	SER	B1357	25.506	-12.337	4.706	1.00	65.96	B
6456	OG	SER	B1357	26.346	-12.987	5.705	1.00	67.36	B
6457	C	SER	B1357	25.462	-14.532	3.415	1.00	68.56	B
6458	O	SER	B1357	26.676	-14.595	3.685	1.00	71.48	B
6459	N	LYS	B1358	24.852	-15.527	2.789	1.00	66.55	B
6460	CA	LYS	B1358	25.605	-16.780	2.602	1.00	65.56	B
6461	CB	LYS	B1358	24.769	-17.723	1.723	1.00	66.86	B
6462	CG	LYS	B1358	24.552	-17.312	0.195	1.00	61.22	B
6463	CD	LYS	B1358	23.806	-16.018	0.065	1.00	59.19	B
6464	CE	LYS	B1358	23.096	-15.992	-1.216	1.00	58.54	B
6465	NZ	LYS	B1358	23.793	-15.306	-2.398	1.00	57.16	B
6466	C	LYS	B1358	27.079	-16.923	2.157	1.00	66.01	B
6467	O	LYS	B1358	27.907	-15.994	1.906	1.00	63.35	B
6468	N	LYS	B1359	27.423	-18.183	2.006	1.00	68.34	B
6469	CA	LYS	B1359	28.795	-18.411	1.558	1.00	70.85	B
6470	CB	LYS	B1359	29.121	-19.871	1.222	1.00	71.21	B
6471	CG	LYS	B1359	29.961	-20.534	2.464	1.00	74.41	B
6472	CD	LYS	B1359	31.573	-20.399	2.294	1.00	78.71	B
6473	CE	LYS	B1359	32.174	-18.830	2.362	1.00	82.41	B
6474	NZ	LYS	B1359	31.999	-17.976	3.678	1.00	74.92	B
6475	C	LYS	B1359	29.204	-17.436	0.509	1.00	70.72	B
6476	O	LYS	B1359	30.365	-17.151	0.452	1.00	72.18	B
6477	N	ASN	B1360	28.228	-16.918	-0.261	1.00	72.16	B
6478	CA	ASN	B1360	28.352	-15.916	-1.397	1.00	72.47	B
6479	CB	ASN	B1360	27.004	-15.928	-2.198	1.00	72.06	B
6480	CG	ASN	B1360	26.649	-14.574	-2.998	1.00	71.47	B
6481	OD1	ASN	B1360	27.314	-13.539	-2.925	1.00	73.12	B
6482	ND2	ASN	B1360	25.578	-14.642	-3.776	1.00	68.16	B
6483	C	ASN	B1360	28.719	-14.519	-0.766	1.00	72.96	B

6484	O	ASN	B1360	29.748	-13.810	-1.156	1.00	72.10	B
6485	N	GLY	B1361	27.944	-14.237	0.304	1.00	71.97	B
6486	CA	GLY	B1361	27.980	-12.986	1.049	1.00	70.10	B
6487	C	GLY	B1361	26.730	-12.148	0.706	1.00	68.12	B
6488	O	GLY	B1361	26.355	-11.297	1.414	1.00	67.91	B
6489	N	GLN	B1362	26.122	-12.318	-0.458	1.00	67.50	B
6490	CA	GLN	B1362	24.958	-11.520	-0.856	1.00	64.62	B
6491	CB	GLN	B1362	24.360	-12.005	-2.215	1.00	63.16	B
6492	CG	GLN	B1362	22.941	-11.407	-2.547	1.00	64.07	B
6493	CD	GLN	B1362	21.853	-12.415	-2.948	1.00	65.05	B
6494	OE1	GLN	B1362	20.686	-12.056	-3.210	1.00	61.54	B
6495	NE2	GLN	B1362	22.244	-13.691	-3.039	1.00	69.55	B
6496	C	GLN	B1362	24.061	-11.930	0.271	1.00	63.28	B
6497	O	GLN	B1362	23.514	-13.042	0.261	1.00	61.85	B
6498	N	LEU	B1363	23.922	-11.036	1.232	1.00	62.35	B
6499	CA	LEU	B1363	22.855	-11.148	2.233	1.00	61.69	B
6500	CB	LEU	B1363	22.576	-9.833	2.959	1.00	59.69	B
6501	CG	LEU	B1363	22.146	-8.607	2.188	1.00	53.63	B
6502	CD1	LEU	B1363	20.886	-7.869	2.584	1.00	48.40	B
6503	CD2	LEU	B1363	23.342	-7.745	2.503	1.00	51.96	B
6504	C	LEU	B1363	21.566	-11.567	1.529	1.00	63.43	B
6505	O	LEU	B1363	21.422	-11.216	0.304	1.00	64.91	B
6506	N	ALA	B1364	20.663	-12.313	2.218	1.00	61.95	B
6507	CA	ALA	B1364	19.413	-12.660	1.562	1.00	62.92	B
6508	CB	ALA	B1364	19.575	-13.724	0.388	1.00	62.94	B
6509	C	ALA	B1364	18.571	-13.201	2.650	1.00	64.49	B
6510	O	ALA	B1364	19.070	-13.400	3.803	1.00	65.76	B
6511	N	ALA	B1365	17.312	-13.449	2.271	1.00	62.59	B
6512	CA	ALA	B1365	16.309	-13.895	3.130	1.00	62.06	B
6513	CB	ALA	B1365	15.027	-13.261	2.685	1.00	63.42	B
6514	C	ALA	B1365	16.098	-15.355	2.944	1.00	63.05	B
6515	O	ALA	B1365	14.937	-15.733	2.874	1.00	63.39	B
6516	N	SER	B1366	17.118	-16.209	2.857	1.00	64.03	B
6517	CA	SER	B1366	16.750	-17.649	2.604	1.00	66.29	B
6518	CB	SER	B1366	17.796	-18.585	1.915	1.00	64.24	B
6519	OG	SER	B1366	18.512	-17.938	0.919	1.00	69.06	B
6520	C	SER	B1366	16.403	-18.447	3.832	1.00	67.03	B
6521	O	SER	B1366	16.314	-19.697	3.643	1.00	66.65	B
6522	N	VAL	B1367	16.315	-17.808	5.037	1.00	67.51	B
6523	CA	VAL	B1367	16.152	-18.552	6.343	1.00	66.80	B
6524	CB	VAL	B1367	17.476	-18.501	7.225	1.00	69.16	B
6525	CG1	VAL	B1367	18.700	-19.207	6.518	1.00	61.97	B
6526	CG2	VAL	B1367	17.737	-17.041	7.915	1.00	67.36	B
6527	C	VAL	B1367	14.904	-18.205	7.199	1.00	67.03	B
6528	O	VAL	B1367	14.151	-17.284	6.801	1.00	69.26	B
6529	N	GLU	B1368	14.653	-18.875	8.348	1.00	65.05	B
6530	CA	GLU	B1368	13.471	-18.506	9.204	1.00	63.32	B
6531	CB	GLU	B1368	12.216	-19.241	8.834	1.00	62.42	B
6532	CG	GLU	B1368	11.488	-18.690	7.703	1.00	63.51	B
6533	CD	GLU	B1368	10.192	-19.422	7.563	1.00	65.60	B
6534	OE1	GLU	B1368	10.178	-20.668	7.934	1.00	67.58	B
6535	OE2	GLU	B1368	9.193	-18.778	7.150	1.00	61.79	B
6536	C	GLU	B1368	13.575	-18.420	10.738	1.00	62.61	B
6537	O	GLU	B1368	12.550	-18.232	11.427	1.00	62.74	B
6538	N	THR	B1369	14.793	-18.540	11.218	1.00	62.23	B
6539	CA	THR	B1369	15.180	-18.549	12.625	1.00	62.47	B

6540	CB	THR	B1369	15.470	-20.007	13.178	1.00	61.44	B
6541	OG1	THR	B1369	16.584	-20.495	12.463	1.00	58.73	B
6542	CG2	THR	B1369	14.276	-20.970	13.170	1.00	54.85	B
6543	C	THR	B1369	16.506	-17.674	12.898	1.00	64.24	B
6544	O	THR	B1369	17.632	-18.054	12.680	1.00	61.95	B
6545	N	ALA	B1370	16.364	-16.518	13.469	1.00	68.50	B
6546	CA	ALA	B1370	17.567	-15.874	14.093	1.00	71.99	B
6547	CB	ALA	B1370	17.127	-15.044	15.448	1.00	71.75	B
6548	C	ALA	B1370	18.777	-16.779	14.386	1.00	72.34	B
6549	O	ALA	B1370	19.008	-17.213	15.546	1.00	74.16	B
6550	N	GLY	B1371	19.587	-17.043	13.385	1.00	72.53	B
6551	CA	GLY	B1371	20.600	-18.045	13.684	1.00	73.95	B
6552	C	GLY	B1371	21.620	-17.393	14.628	1.00	73.61	B
6553	O	GLY	B1371	21.713	-17.668	15.844	1.00	71.24	B
6554	N	ASP	B1372	22.353	-16.468	14.017	1.00	73.47	B
6555	CA	ASP	B1372	23.454	-15.844	14.680	1.00	73.16	B
6556	CB	ASP	B1372	24.270	-16.963	15.459	1.00	72.79	B
6557	CG	ASP	B1372	25.706	-16.511	15.869	1.00	71.45	B
6558	OD1	ASP	B1372	26.581	-17.381	16.072	1.00	64.97	B
6559	OD2	ASP	B1372	25.957	-15.278	15.932	1.00	70.36	B
6560	C	ASP	B1372	24.115	-15.226	13.469	1.00	72.58	B
6561	O	ASP	B1372	24.934	-14.324	13.514	1.00	74.52	B
6562	N	SER	B1373	23.752	-15.809	12.371	1.00	72.73	B
6563	CA	SER	B1373	24.302	-15.525	11.114	1.00	71.68	B
6564	CB	SER	B1373	24.114	-16.785	10.224	1.00	72.31	B
6565	OG	SER	B1373	25.079	-17.814	10.356	1.00	70.43	B
6566	C	SER	B1373	23.277	-14.543	10.572	1.00	71.30	B
6567	O	SER	B1373	23.581	-13.885	9.555	1.00	73.55	B
6568	N	GLU	B1374	22.042	-14.537	11.146	1.00	67.27	B
6569	CA	GLU	B1374	20.859	-13.925	10.473	1.00	62.03	B
6570	CB	GLU	B1374	19.664	-14.750	10.766	1.00	62.47	B
6571	CG	GLU	B1374	19.272	-15.575	9.614	1.00	59.42	B
6572	CD	GLU	B1374	20.410	-16.385	9.071	1.00	63.76	B
6573	OE1	GLU	B1374	21.659	-16.123	9.482	1.00	53.57	B
6574	OE2	GLU	B1374	19.980	-17.237	8.191	1.00	52.31	B
6575	C	GLU	B1374	20.576	-12.539	11.017	1.00	59.87	B
6576	O	GLU	B1374	19.459	-11.967	10.923	1.00	55.51	B
6577	N	LEU	B1375	21.662	-12.018	11.535	1.00	57.78	B
6578	CA	LEU	B1375	21.647	-11.030	12.561	1.00	58.72	B
6579	CB	LEU	B1375	21.954	-11.705	13.917	1.00	57.99	B
6580	CG	LEU	B1375	21.147	-12.773	14.652	1.00	47.91	B
6581	CD1	LEU	B1375	22.080	-13.415	15.427	1.00	51.60	B
6582	CD2	LEU	B1375	20.296	-12.376	15.598	1.00	34.02	B
6583	C	LEU	B1375	22.837	-10.142	12.174	1.00	59.81	B
6584	O	LEU	B1375	23.932	-10.677	11.804	1.00	63.60	B
6585	N	PHE	B1376	22.698	-8.816	12.227	1.00	57.81	B
6586	CA	PHE	B1376	23.753	-8.052	11.637	1.00	53.63	B
6587	CB	PHE	B1376	23.433	-7.388	10.285	1.00	52.93	B
6588	CG	PHE	B1376	22.426	-8.030	9.490	1.00	50.52	B
6589	CD1	PHE	B1376	21.135	-8.239	9.992	1.00	50.08	B
6590	CD2	PHE	B1376	22.748	-8.411	8.170	1.00	52.56	B
6591	CE1	PHE	B1376	20.108	-8.848	9.140	1.00	57.55	B
6592	CE2	PHE	B1376	21.745	-8.988	7.271	1.00	56.27	B
6593	CZ	PHE	B1376	20.430	-9.253	7.723	1.00	51.85	B
6594	C	PHE	B1376	23.844	-6.981	12.593	1.00	52.46	B
6595	O	PHE	B1376	22.857	-6.597	13.119	1.00	51.28	B

6596	N	LEU	B1377	25.061	-6.469	12.661	1.00	52.83	B
6597	CA	LEU	B1377	25.506	-5.377	13.374	1.00	52.41	B
6598	CB	LEU	B1377	26.964	-5.614	13.576	1.00	50.98	B
6599	CG	LEU	B1377	27.412	-4.440	14.357	1.00	49.39	B
6600	CD1	LEU	B1377	26.529	-4.440	15.537	1.00	56.86	B
6601	CD2	LEU	B1377	28.782	-4.808	14.828	1.00	49.33	B
6602	C	LEU	B1377	25.196	-4.099	12.584	1.00	55.48	B
6603	O	LEU	B1377	25.046	-4.043	11.268	1.00	55.53	B
6604	N	MET	B1378	24.972	-3.072	13.424	1.00	56.40	B
6605	CA	MET	B1378	24.419	-1.780	12.991	1.00	54.70	B
6606	CB	MET	B1378	23.068	-1.572	13.515	1.00	52.97	B
6607	CG	MET	B1378	21.943	-1.462	12.394	1.00	56.09	B
6608	SD	MET	B1378	20.662	-0.026	12.413	1.00	55.66	B
6609	CE	MET	B1378	21.184	0.793	14.006	1.00	37.57	B
6610	C	MET	B1378	25.344	-0.866	13.698	1.00	55.81	B
6611	O	MET	B1378	25.641	-1.069	14.953	1.00	53.53	B
6612	N	LYS	B1379	25.857	0.118	12.898	1.00	55.79	B
6613	CA	LYS	B1379	26.674	1.197	13.508	1.00	54.95	B
6614	CB	LYS	B1379	28.151	0.820	13.337	1.00	56.76	B
6615	CG	LYS	B1379	29.327	1.862	13.635	1.00	54.51	B
6616	CD	LYS	B1379	30.611	1.186	13.111	1.00	52.16	B
6617	CE	LYS	B1379	31.803	2.009	13.297	1.00	50.99	B
6618	NZ	LYS	B1379	33.117	1.270	13.066	1.00	45.15	B
6619	C	LYS	B1379	26.315	2.546	12.884	1.00	55.02	B
6620	O	LYS	B1379	26.473	2.716	11.698	1.00	56.78	B
6621	N	LEU	B1380	25.873	3.492	13.690	1.00	52.18	B
6622	CA	LEU	B1380	25.411	4.801	13.215	1.00	51.40	B
6623	CB	LEU	B1380	24.404	5.430	14.216	1.00	49.93	B
6624	CG	LEU	B1380	23.490	6.611	14.537	1.00	48.50	B
6625	CD1	LEU	B1380	23.529	7.426	15.910	1.00	43.88	B
6626	CD2	LEU	B1380	23.226	7.538	13.505	1.00	53.16	B
6627	C	LEU	B1380	26.643	5.595	13.159	1.00	52.10	B
6628	O	LEU	B1380	27.282	5.960	14.250	1.00	55.89	B
6629	N	ILE	B1381	26.976	5.950	11.915	1.00	49.70	B
6630	CA	ILE	B1381	28.262	6.531	11.584	1.00	46.77	B
6631	CB	ILE	B1381	28.802	5.879	10.338	1.00	46.38	B
6632	CG2	ILE	B1381	29.423	4.531	10.651	1.00	38.23	B
6633	CG1	ILE	B1381	27.694	5.815	9.215	1.00	45.60	B
6634	CD1	ILE	B1381	28.345	5.996	7.804	1.00	44.84	B
6635	C	ILE	B1381	28.098	8.021	11.336	1.00	49.17	B
6636	O	ILE	B1381	29.042	8.831	11.103	1.00	49.72	B
6637	N	ASN	B1382	26.887	8.459	11.491	1.00	51.76	B
6638	CA	ASN	B1382	26.668	9.901	11.415	1.00	54.39	B
6639	CB	ASN	B1382	25.788	10.231	10.182	1.00	53.13	B
6640	CG	ASN	B1382	24.285	10.124	10.477	1.00	58.65	B
6641	OD1	ASN	B1382	23.874	9.195	11.232	1.00	60.21	B
6642	ND2	ASN	B1382	23.422	11.137	9.919	1.00	55.37	B
6643	C	ASN	B1382	26.200	10.628	12.675	1.00	54.03	B
6644	O	ASN	B1382	25.572	11.645	12.544	1.00	57.36	B
6645	N	ARG	B1383	26.469	10.132	13.873	1.00	53.79	B
6646	CA	ARG	B1383	26.188	10.944	15.130	1.00	52.38	B
6647	CB	ARG	B1383	24.807	10.778	15.785	1.00	46.51	B
6648	CG	ARG	B1383	23.800	11.424	15.055	1.00	40.39	B
6649	CD	ARG	B1383	23.057	12.595	15.609	1.00	39.99	B
6650	NE	ARG	B1383	21.801	13.038	14.867	1.00	41.31	B
6651	CZ	ARG	B1383	21.713	13.301	13.520	1.00	34.32	B

6652	NH1	ARG	B1383	22.751	13.018	12.769	1.00	31.86	B
6653	NH2	ARG	B1383	20.625	13.769	12.907	1.00	33.69	B
6654	C	ARG	B1383	27.201	10.587	16.188	1.00	54.24	B
6655	O	ARG	B1383	26.844	10.084	17.232	1.00	55.64	B
6656	N	PRO	B1384	28.458	10.899	15.934	1.00	55.27	B
6657	CD	PRO	B1384	29.055	11.140	14.604	1.00	56.95	B
6658	CA	PRO	B1384	29.405	11.052	17.031	1.00	53.59	B
6659	CB	PRO	B1384	30.700	10.787	16.359	1.00	55.05	B
6660	CG	PRO	B1384	30.576	11.305	14.950	1.00	57.24	B
6661	C	PRO	B1384	29.325	12.412	17.844	1.00	53.25	B
6662	O	PRO	B1384	29.934	12.515	18.932	1.00	53.67	B
6663	N	ILE	B1385	28.463	13.378	17.513	1.00	52.22	B
6664	CA	ILE	B1385	27.994	14.209	18.661	1.00	51.01	B
6665	CB	ILE	B1385	28.336	15.645	18.578	1.00	50.87	B
6666	CG2	ILE	B1385	27.954	16.400	19.946	1.00	49.32	B
6667	CG1	ILE	B1385	29.615	15.993	17.789	1.00	49.53	B
6668	CD1	ILE	B1385	31.001	15.491	18.234	1.00	54.91	B
6669	C	ILE	B1385	26.453	14.315	18.770	1.00	51.82	B
6670	O	ILE	B1385	25.749	14.496	17.774	1.00	54.22	B
6671	N	ILE	B1386	25.918	14.312	19.974	1.00	49.03	B
6672	CA	ILE	B1386	24.528	13.969	20.123	1.00	48.33	B
6673	CB	ILE	B1386	24.215	12.568	20.645	1.00	48.81	B
6674	CG2	ILE	B1386	22.800	12.135	20.282	1.00	51.96	B
6675	CG1	ILE	B1386	25.114	11.597	19.996	1.00	53.54	B
6676	CD1	ILE	B1386	26.135	11.223	21.012	1.00	69.11	B
6677	C	ILE	B1386	23.849	14.856	21.091	1.00	45.72	B
6678	O	ILE	B1386	24.412	15.325	22.042	1.00	44.28	B
6679	N	VAL	B1387	22.595	15.036	20.747	1.00	41.43	B
6680	CA	VAL	B1387	21.865	15.956	21.343	1.00	41.38	B
6681	CB	VAL	B1387	21.651	17.063	20.431	1.00	41.36	B
6682	CG1	VAL	B1387	20.364	17.834	20.935	1.00	39.46	B
6683	CG2	VAL	B1387	22.906	17.947	20.457	1.00	38.90	B
6684	C	VAL	B1387	20.657	15.122	21.406	1.00	42.06	B
6685	O	VAL	B1387	20.402	14.502	20.428	1.00	42.08	B
6686	N	PHE	B1388	19.941	15.113	22.543	1.00	41.24	B
6687	CA	PHE	B1388	18.874	14.323	22.694	1.00	45.93	B
6688	CB	PHE	B1388	19.022	13.331	23.883	1.00	47.17	B
6689	CG	PHE	B1388	20.049	12.240	23.712	1.00	46.86	B
6690	CD1	PHE	B1388	19.820	11.142	22.864	1.00	41.85	B
6691	CD2	PHE	B1388	21.234	12.345	24.295	1.00	44.67	B
6692	CE1	PHE	B1388	20.679	10.212	22.682	1.00	36.98	B
6693	CE2	PHE	B1388	22.145	11.292	24.052	1.00	53.99	B
6694	CZ	PHE	B1388	21.845	10.226	23.260	1.00	42.41	B
6695	C	PHE	B1388	17.782	15.306	23.091	1.00	49.86	B
6696	O	PHE	B1388	17.814	15.842	24.180	1.00	46.59	B
6697	N	ARG	B1389	16.702	15.402	22.244	1.00	55.44	B
6698	CA	ARG	B1389	15.409	16.087	22.608	1.00	54.29	B
6699	CB	ARG	B1389	15.099	16.920	21.433	1.00	53.25	B
6700	CG	ARG	B1389	14.090	17.986	21.754	1.00	55.97	B
6701	CD	ARG	B1389	12.711	17.675	21.176	1.00	51.33	B
6702	NE	ARG	B1389	11.892	18.843	21.323	1.00	63.58	B
6703	CZ	ARG	B1389	12.026	20.016	20.659	1.00	71.68	B
6704	NH1	ARG	B1389	12.965	20.280	19.708	1.00	77.76	B
6705	NH2	ARG	B1389	11.159	20.959	20.958	1.00	72.28	B
6706	C	ARG	B1389	14.199	15.200	23.067	1.00	55.51	B
6707	O	ARG	B1389	13.915	14.154	22.465	1.00	59.39	B

6708	N	GLY	B1390	13.447	15.554	24.105	1.00	54.11	B
6709	CA	GLY	B1390	12.307	14.726	24.410	1.00	53.67	B
6710	C	GLY	B1390	11.083	15.535	24.570	1.00	56.87	B
6711	O	GLY	B1390	11.193	16.806	24.428	1.00	60.20	B
6712	N	GLU	B1391	9.979	14.853	24.960	1.00	57.51	B
6713	CA	GLU	B1391	8.613	15.416	25.126	1.00	60.57	B
6714	CB	GLU	B1391	7.537	14.322	25.484	1.00	60.91	B
6715	CG	GLU	B1391	6.856	14.488	26.953	1.00	60.55	B
6716	CD	GLU	B1391	5.485	13.727	27.199	1.00	59.22	B
6717	OE1	GLU	B1391	5.326	12.594	26.832	1.00	55.43	B
6718	OE2	GLU	B1391	4.512	14.239	27.752	1.00	59.90	B
6719	C	GLU	B1391	8.340	16.459	26.146	1.00	63.69	B
6720	O	GLU	B1391	7.137	16.792	26.355	1.00	65.96	B
6721	N	HIS	B1392	9.346	16.865	26.901	1.00	65.54	B
6722	CA	HIS	B1392	9.244	18.069	27.799	1.00	66.53	B
6723	CB	HIS	B1392	8.807	17.705	29.295	1.00	65.26	B
6724	CG	HIS	B1392	7.359	17.291	29.527	1.00	61.22	B
6725	CD2	HIS	B1392	6.826	16.083	29.787	1.00	57.18	B
6726	ND1	HIS	B1392	6.311	18.197	29.713	1.00	62.21	B
6727	CE1	HIS	B1392	5.176	17.563	29.986	1.00	53.09	B
6728	NE2	HIS	B1392	5.465	16.269	30.007	1.00	58.41	B
6729	C	HIS	B1392	10.679	18.677	28.007	1.00	67.34	B
6730	O	HIS	B1392	10.860	19.272	29.033	1.00	66.90	B
6731	N	GLY	B1393	11.728	18.436	27.185	1.00	68.35	B
6732	CA	GLY	B1393	13.025	19.206	27.400	1.00	69.36	B
6733	C	GLY	B1393	14.154	18.586	26.597	1.00	71.18	B
6734	O	GLY	B1393	13.845	17.683	25.825	1.00	74.70	B
6735	N	PHE	B1394	15.423	19.003	26.746	1.00	68.74	B
6736	CA	PHE	B1394	16.571	18.226	26.210	1.00	67.22	B
6737	CB	PHE	B1394	17.526	19.148	25.452	1.00	69.16	B
6738	CG	PHE	B1394	16.797	19.979	24.427	1.00	72.33	B
6739	CD1	PHE	B1394	15.691	20.843	24.864	1.00	71.36	B
6740	CD2	PHE	B1394	17.093	19.849	23.089	1.00	69.77	B
6741	CE1	PHE	B1394	14.969	21.561	24.011	1.00	68.26	B
6742	CE2	PHE	B1394	16.306	20.541	22.192	1.00	76.72	B
6743	CZ	PHE	B1394	15.260	21.425	22.637	1.00	72.29	B
6744	C	PHE	B1394	17.315	17.283	27.190	1.00	66.16	B
6745	O	PHE	B1394	16.767	16.949	28.189	1.00	65.99	B
6746	N	ILE	B1395	18.504	16.762	26.902	1.00	63.93	B
6747	CA	ILE	B1395	19.032	15.932	27.904	1.00	64.26	B
6748	CB	ILE	B1395	19.261	14.407	27.535	1.00	64.90	B
6749	CG2	ILE	B1395	19.912	13.664	28.752	1.00	62.07	B
6750	CG1	ILE	B1395	18.038	13.642	27.213	1.00	61.51	B
6751	CD1	ILE	B1395	18.371	12.250	26.641	1.00	61.42	B
6752	C	ILE	B1395	20.403	16.428	28.179	1.00	66.56	B
6753	O	ILE	B1395	21.266	16.210	27.335	1.00	66.32	B
6754	N	GLY	B1396	20.661	17.009	29.363	1.00	67.38	B
6755	CA	GLY	B1396	22.056	17.541	29.619	1.00	66.81	B
6756	C	GLY	B1396	22.375	17.442	31.060	1.00	66.26	B
6757	O	GLY	B1396	21.447	17.590	31.839	1.00	68.36	B
6758	N	CYS	B1397	23.616	17.116	31.447	1.00	66.10	B
6759	CA	CYS	B1397	24.007	17.171	32.875	1.00	64.23	B
6760	CB	CYS	B1397	25.503	17.115	33.101	1.00	62.89	B
6761	SG	CYS	B1397	26.606	15.982	32.159	1.00	64.20	B
6762	C	CYS	B1397	23.715	18.514	33.394	1.00	63.64	B
6763	O	CYS	B1397	24.514	19.333	33.281	1.00	65.22	B

6764	N	ARG	B1398	22.593	18.767	33.981	1.00	66.40	B
6765	CA	ARG	B1398	22.479	19.939	34.794	1.00	69.57	B
6766	CB	ARG	B1398	21.234	19.875	35.682	1.00	69.46	B
6767	CG	ARG	B1398	21.013	21.210	36.438	1.00	67.76	B
6768	CD	ARG	B1398	21.267	20.939	37.861	1.00	63.75	B
6769	NE	ARG	B1398	20.244	20.239	38.668	1.00	50.30	B
6770	CZ	ARG	B1398	20.598	19.334	39.579	1.00	55.98	B
6771	NH1	ARG	B1398	21.893	18.966	39.631	1.00	58.49	B
6772	NH2	ARG	B1398	19.706	18.708	40.379	1.00	54.57	B
6773	C	ARG	B1398	23.776	20.125	35.651	1.00	73.35	B
6774	O	ARG	B1398	24.272	19.112	36.376	1.00	70.82	B
6775	N	LYS	B1399	24.335	21.379	35.533	1.00	75.68	B
6776	CA	LYS	B1399	25.399	21.810	36.425	1.00	77.56	B
6777	CB	LYS	B1399	24.772	21.874	37.839	1.00	77.72	B
6778	CG	LYS	B1399	25.198	22.955	38.822	1.00	75.53	B
6779	CD	LYS	B1399	24.183	24.086	38.819	1.00	75.80	B
6780	CE	LYS	B1399	23.025	24.062	39.927	1.00	69.74	B
6781	NZ	LYS	B1399	23.047	25.602	40.334	1.00	65.43	B
6782	C	LYS	B1399	26.526	20.719	36.344	1.00	79.43	B
6783	O	LYS	B1399	26.889	20.184	35.182	1.00	81.18	B
6784	N	VAL	B1400	27.073	20.343	37.532	1.00	80.05	B
6785	CA	VAL	B1400	28.323	19.440	37.665	1.00	79.11	B
6786	CB	VAL	B1400	29.666	20.302	37.566	1.00	79.48	B
6787	CG1	VAL	B1400	29.696	21.293	36.312	1.00	67.15	B
6788	CG2	VAL	B1400	29.835	21.098	38.930	1.00	81.72	B
6789	C	VAL	B1400	28.200	18.485	38.952	1.00	80.57	B
6790	O	VAL	B1400	29.152	17.838	39.539	1.00	80.14	B
6791	N	THR	B1401	26.928	18.405	39.316	1.00	81.55	B
6792	CA	THR	B1401	26.364	17.554	40.372	1.00	81.00	B
6793	CB	THR	B1401	24.807	18.002	40.696	1.00	82.08	B
6794	OG1	THR	B1401	24.667	19.475	40.697	1.00	74.51	B
6795	CG2	THR	B1401	24.206	17.292	42.038	1.00	81.33	B
6796	C	THR	B1401	26.611	16.090	39.919	1.00	80.22	B
6797	O	THR	B1401	26.438	15.121	40.701	1.00	80.99	B
6798	N	GLY	B1402	27.170	15.985	38.705	1.00	78.16	B
6799	CA	GLY	B1402	27.466	14.705	38.010	1.00	74.94	B
6800	C	GLY	B1402	26.155	14.343	37.317	1.00	73.55	B
6801	O	GLY	B1402	26.199	13.821	36.182	1.00	71.93	B
6802	N	THR	B1403	25.031	14.646	38.062	1.00	70.35	B
6803	CA	THR	B1403	23.650	14.408	37.678	1.00	67.26	B
6804	CB	THR	B1403	22.542	14.836	38.842	1.00	69.11	B
6805	OG1	THR	B1403	22.069	16.175	38.707	1.00	64.57	B
6806	CG2	THR	B1403	23.023	14.526	40.356	1.00	68.24	B
6807	C	THR	B1403	23.310	14.775	36.163	1.00	65.20	B
6808	O	THR	B1403	24.128	15.336	35.521	1.00	63.01	B
6809	N	LEU	B1404	22.141	14.354	35.647	1.00	63.61	B
6810	CA	LEU	B1404	21.773	14.243	34.198	1.00	63.06	B
6811	CB	LEU	B1404	22.207	12.840	33.632	1.00	62.98	B
6812	CG	LEU	B1404	22.634	12.647	32.110	1.00	59.28	B
6813	CD1	LEU	B1404	23.221	13.885	31.661	1.00	54.35	B
6814	CD2	LEU	B1404	23.589	11.585	31.832	1.00	57.47	B
6815	C	LEU	B1404	20.234	14.500	33.908	1.00	64.16	B
6816	O	LEU	B1404	19.366	13.647	34.164	1.00	64.66	B
6817	N	ASP	B1405	19.848	15.670	33.395	1.00	64.15	B
6818	CA	ASP	B1405	18.429	15.945	33.343	1.00	63.74	B
6819	CB	ASP	B1405	18.172	17.255	34.079	1.00	64.91	B

6820	CG	ASP	B1405	18.211	17.087	35.612	1.00	65.49	B
6821	OD1	ASP	B1405	19.380	17.027	36.128	1.00	64.78	B
6822	OD2	ASP	B1405	17.083	17.027	36.237	1.00	62.42	B
6823	C	ASP	B1405	17.794	15.878	31.929	1.00	63.68	B
6824	O	ASP	B1405	18.504	15.977	30.906	1.00	63.81	B
6825	N	ALA	B1406	16.474	15.715	31.909	1.00	63.20	B
6826	CA	ALA	B1406	15.671	15.394	30.712	1.00	64.80	B
6827	CB	ALA	B1406	14.614	14.333	30.988	1.00	63.22	B
6828	C	ALA	B1406	14.956	16.620	30.303	1.00	65.08	B
6829	O	ALA	B1406	14.816	16.933	29.143	1.00	66.36	B
6830	N	ASN	B1407	14.435	17.330	31.256	1.00	67.23	B
6831	CA	ASN	B1407	13.737	18.572	30.868	1.00	66.03	B
6832	CB	ASN	B1407	12.740	19.033	31.943	1.00	66.91	B
6833	CG	ASN	B1407	13.282	18.944	33.291	1.00	64.18	B
6834	OD1	ASN	B1407	12.548	19.057	34.269	1.00	66.28	B
6835	ND2	ASN	B1407	14.601	18.777	33.369	1.00	61.30	B
6836	C	ASN	B1407	14.535	19.761	30.497	1.00	64.47	B
6837	O	ASN	B1407	13.874	20.741	30.277	1.00	64.37	B
6838	N	ARG	B1408	15.884	19.720	30.430	1.00	62.96	B
6839	CA	ARG	B1408	16.608	21.001	30.333	1.00	63.40	B
6840	CB	ARG	B1408	18.121	21.001	30.044	1.00	64.00	B
6841	CG	ARG	B1408	18.776	19.671	30.304	1.00	68.91	B
6842	CD	ARG	B1408	19.740	19.697	31.404	1.00	67.03	B
6843	NE	ARG	B1408	19.602	20.814	32.274	1.00	66.75	B
6844	CZ	ARG	B1408	20.649	21.423	32.847	1.00	75.82	B
6845	NH1	ARG	B1408	20.413	22.447	33.674	1.00	81.34	B
6846	NH2	ARG	B1408	21.939	21.060	32.586	1.00	74.13	B
6847	C	ARG	B1408	16.014	21.487	29.132	1.00	61.84	B
6848	O	ARG	B1408	15.673	20.669	28.287	1.00	63.01	B
6849	N	SER	B1409	15.779	22.806	29.152	1.00	61.52	B
6850	CA	SER	B1409	15.485	23.735	28.078	1.00	60.25	B
6851	CB	SER	B1409	15.139	25.075	28.719	1.00	61.22	B
6852	OG	SER	B1409	13.805	25.130	29.264	1.00	59.91	B
6853	C	SER	B1409	16.658	24.018	27.067	1.00	60.03	B
6854	O	SER	B1409	16.475	24.761	26.067	1.00	60.01	B
6855	N	SER	B1410	17.812	23.356	27.277	1.00	58.69	B
6856	CA	SER	B1410	18.989	23.523	26.463	1.00	55.42	B
6857	CB	SER	B1410	19.645	24.779	26.990	1.00	55.33	B
6858	OG	SER	B1410	18.537	25.646	27.282	1.00	52.22	B
6859	C	SER	B1410	19.866	22.328	26.684	1.00	55.28	B
6860	O	SER	B1410	19.681	21.671	27.754	1.00	57.88	B
6861	N	TYR	B1411	20.839	22.115	25.783	1.00	51.35	B
6862	CA	TYR	B1411	21.244	20.811	25.302	1.00	49.49	B
6863	CB	TYR	B1411	21.288	20.671	23.744	1.00	52.91	B
6864	CG	TYR	B1411	20.812	21.880	22.880	1.00	56.18	B
6865	CD1	TYR	B1411	21.553	22.321	21.819	1.00	56.32	B
6866	CE1	TYR	B1411	21.137	23.394	21.110	1.00	55.60	B
6867	CD2	TYR	B1411	19.604	22.589	23.213	1.00	63.48	B
6868	CE2	TYR	B1411	19.188	23.659	22.515	1.00	56.75	B
6869	CZ	TYR	B1411	19.935	24.049	21.455	1.00	53.66	B
6870	OH	TYR	B1411	19.454	25.116	20.734	1.00	44.04	B
6871	C	TYR	B1411	22.605	20.813	25.555	1.00	49.11	B
6872	O	TYR	B1411	23.154	21.885	25.673	1.00	51.98	B
6873	N	ASP	B1412	23.227	19.655	25.570	1.00	46.77	B
6874	CA	ASP	B1412	24.573	19.685	25.967	1.00	47.34	B
6875	CB	ASP	B1412	24.803	19.108	27.376	1.00	48.19	B

6876	CG	ASP	B1412	24.072	19.834	28.501	1.00	53.85	B
6877	OD1	ASP	B1412	23.848	19.106	29.556	1.00	55.84	B
6878	OD2	ASP	B1412	23.707	21.089	28.364	1.00	47.87	B
6879	C	ASP	B1412	25.219	18.808	24.939	1.00	47.32	B
6880	O	ASP	B1412	24.908	17.696	24.628	1.00	46.52	B
6881	N	VAL	B1413	26.208	19.295	24.351	1.00	49.13	B
6882	CA	VAL	B1413	26.679	18.427	23.356	1.00	50.81	B
6883	CB	VAL	B1413	27.457	19.237	22.319	1.00	47.92	B
6884	CG1	VAL	B1413	28.647	18.478	21.913	1.00	46.74	B
6885	CG2	VAL	B1413	26.522	19.436	21.194	1.00	46.02	B
6886	C	VAL	B1413	27.375	17.103	24.033	1.00	53.46	B
6887	O	VAL	B1413	28.525	17.135	24.638	1.00	53.97	B
6888	N	PHE	B1414	26.703	15.964	23.971	1.00	53.56	B
6889	CA	PHE	B1414	27.363	14.840	24.591	1.00	56.16	B
6890	CB	PHE	B1414	26.417	13.792	25.153	1.00	55.21	B
6891	CG	PHE	B1414	25.654	14.271	26.374	1.00	52.11	B
6892	CD1	PHE	B1414	26.292	14.522	27.502	1.00	49.30	B
6893	CD2	PHE	B1414	24.266	14.425	26.363	1.00	51.29	B
6894	CE1	PHE	B1414	25.549	14.924	28.731	1.00	42.58	B
6895	CE2	PHE	B1414	23.513	14.824	27.520	1.00	46.92	B
6896	CZ	PHE	B1414	24.252	15.086	28.737	1.00	46.43	B
6897	C	PHE	B1414	28.058	14.438	23.394	1.00	56.97	B
6898	O	PHE	B1414	28.109	15.327	22.527	1.00	54.28	B
6899	N	GLN	B1415	28.606	13.202	23.376	1.00	58.61	B
6900	CA	GLN	B1415	29.383	12.648	22.287	1.00	62.27	B
6901	CB	GLN	B1415	30.786	13.286	22.311	1.00	64.29	B
6902	CG	GLN	B1415	32.117	12.538	22.908	1.00	64.66	B
6903	CD	GLN	B1415	33.145	13.647	23.502	1.00	66.50	B
6904	OE1	GLN	B1415	32.775	14.850	23.721	1.00	72.17	B
6905	NE2	GLN	B1415	34.383	13.232	23.791	1.00	65.67	B
6906	C	GLN	B1415	29.507	11.184	22.579	1.00	61.70	B
6907	O	GLN	B1415	29.290	10.848	23.748	1.00	63.48	B
6908	N	LEU	B1416	29.941	10.336	21.617	1.00	60.36	B
6909	CA	LEU	B1416	29.455	8.892	21.567	1.00	58.30	B
6910	CB	LEU	B1416	27.950	8.761	21.277	1.00	58.36	B
6911	CG	LEU	B1416	26.965	8.180	20.214	1.00	61.09	B
6912	CD1	LEU	B1416	27.470	7.247	19.073	1.00	62.22	B
6913	CD2	LEU	B1416	25.779	7.554	20.927	1.00	57.12	B
6914	C	LEU	B1416	30.123	7.923	20.710	1.00	57.89	B
6915	O	LEU	B1416	30.527	8.259	19.605	1.00	59.24	B
6916	N	GLU	B1417	30.137	6.685	21.182	1.00	58.15	B
6917	CA	GLU	B1417	30.875	5.626	20.526	1.00	59.25	B
6918	CB	GLU	B1417	31.773	5.004	21.514	1.00	60.64	B
6919	CG	GLU	B1417	33.228	5.347	21.428	1.00	58.35	B
6920	CD	GLU	B1417	33.704	5.627	22.861	1.00	63.66	B
6921	OE1	GLU	B1417	33.705	4.660	23.730	1.00	60.79	B
6922	OE2	GLU	B1417	33.960	6.869	23.164	1.00	62.00	B
6923	C	GLU	B1417	30.067	4.427	19.983	1.00	60.54	B
6924	O	GLU	B1417	28.807	4.257	20.289	1.00	61.51	B
6925	N	PHE	B1418	30.768	3.558	19.226	1.00	58.81	B
6926	CA	PHE	B1418	30.148	2.272	18.959	1.00	59.30	B
6927	CB	PHE	B1418	30.115	2.071	17.506	1.00	58.10	B
6928	CG	PHE	B1418	29.469	0.897	17.153	1.00	53.26	B
6929	CD1	PHE	B1418	28.154	0.730	17.507	1.00	62.17	B
6930	CD2	PHE	B1418	30.124	-0.100	16.467	1.00	51.96	B
6931	CE1	PHE	B1418	27.387	-0.580	17.061	1.00	66.76	B

6932	CE2	PHE	B1418	29.520	-1.322	16.036	1.00	53.19	B
6933	CZ	PHE	B1418	28.105	-1.574	16.329	1.00	60.13	B
6934	C	PHE	B1418	30.864	1.101	19.681	1.00	61.21	B
6935	O	PHE	B1418	32.101	1.150	19.819	1.00	65.68	B
6936	N	ASN	B1419	30.173	0.054	20.144	1.00	59.31	B
6937	CA	ASN	B1419	30.859	-1.030	20.947	1.00	58.27	B
6938	CB	ASN	B1419	30.629	-0.801	22.499	1.00	59.03	B
6939	CG	ASN	B1419	31.582	-1.657	23.484	1.00	59.36	B
6940	OD1	ASN	B1419	32.578	-1.158	24.051	1.00	53.90	B
6941	ND2	ASN	B1419	31.151	-2.848	23.794	1.00	59.42	B
6942	C	ASN	B1419	30.224	-2.324	20.371	1.00	57.95	B
6943	O	ASN	B1419	29.220	-2.836	20.780	1.00	59.71	B
6944	N	ASP	B1420	30.785	-2.823	19.327	1.00	56.88	B
6945	CA	ASP	B1420	30.375	-4.029	18.794	1.00	55.57	B
6946	CB	ASP	B1420	31.233	-5.122	19.417	1.00	53.59	B
6947	CG	ASP	B1420	31.522	-6.234	18.408	1.00	57.38	B
6948	OD1	ASP	B1420	30.468	-6.920	18.043	1.00	50.17	B
6949	OD2	ASP	B1420	32.742	-6.383	17.950	1.00	50.61	B
6950	C	ASP	B1420	28.790	-4.268	18.535	1.00	56.78	B
6951	O	ASP	B1420	28.321	-5.407	18.136	1.00	56.79	B
6952	N	GLY	B1421	27.993	-3.188	18.672	1.00	55.15	B
6953	CA	GLY	B1421	26.519	-3.311	18.587	1.00	54.75	B
6954	C	GLY	B1421	25.823	-2.409	19.632	1.00	55.33	B
6955	O	GLY	B1421	24.559	-2.364	19.702	1.00	54.17	B
6956	N	ALA	B1422	26.588	-1.636	20.425	1.00	52.97	B
6957	CA	ALA	B1422	25.988	-1.004	21.584	1.00	52.58	B
6958	CB	ALA	B1422	26.310	-1.687	22.804	1.00	48.60	B
6959	C	ALA	B1422	26.589	0.349	21.600	1.00	53.85	B
6960	O	ALA	B1422	27.576	0.565	20.884	1.00	54.20	B
6961	N	TYR	B1423	26.063	1.217	22.491	1.00	53.42	B
6962	CA	TYR	B1423	26.481	2.620	22.540	1.00	51.84	B
6963	CB	TYR	B1423	25.265	3.515	22.004	1.00	50.76	B
6964	CG	TYR	B1423	25.171	3.414	20.454	1.00	46.58	B
6965	CD1	TYR	B1423	24.311	2.505	19.885	1.00	29.54	B
6966	CE1	TYR	B1423	24.198	2.300	18.587	1.00	39.99	B
6967	CD2	TYR	B1423	26.075	4.111	19.608	1.00	39.84	B
6968	CE2	TYR	B1423	25.982	3.891	18.195	1.00	45.77	B
6969	CZ	TYR	B1423	25.042	2.926	17.687	1.00	50.96	B
6970	OH	TYR	B1423	24.900	2.526	16.276	1.00	54.25	B
6971	C	TYR	B1423	27.015	3.127	23.908	1.00	53.05	B
6972	O	TYR	B1423	26.478	2.778	24.956	1.00	53.35	B
6973	N	ASN	B1424	27.957	4.058	23.849	1.00	52.88	B
6974	CA	ASN	B1424	28.509	4.663	24.960	1.00	53.50	B
6975	CB	ASN	B1424	29.962	4.162	25.018	1.00	55.13	B
6976	CG	ASN	B1424	30.154	2.919	25.844	1.00	55.00	B
6977	OD1	ASN	B1424	30.467	1.864	25.303	1.00	57.51	B
6978	ND2	ASN	B1424	30.068	3.067	27.203	1.00	54.98	B
6979	C	ASN	B1424	28.699	6.174	24.816	1.00	53.97	B
6980	O	ASN	B1424	29.525	6.528	24.033	1.00	54.86	B
6981	N	ILE	B1425	28.181	7.028	25.716	1.00	53.97	B
6982	CA	ILE	B1425	28.116	8.472	25.659	1.00	52.60	B
6983	CB	ILE	B1425	26.630	8.683	25.965	1.00	51.24	B
6984	CG2	ILE	B1425	26.237	9.993	26.577	1.00	46.60	B
6985	CG1	ILE	B1425	25.849	8.242	24.815	1.00	46.90	B
6986	CD1	ILE	B1425	24.643	7.497	25.233	1.00	52.62	B
6987	C	ILE	B1425	28.866	8.921	26.910	1.00	56.81	B

6988	O	ILE	B1425	29.095	8.064	27.794	1.00	58.88	B
6989	N	LYS	B1426	29.100	10.267	27.078	1.00	59.55	B
6990	CA	LYS	B1426	30.100	11.012	28.031	1.00	56.37	B
6991	CB	LYS	B1426	31.574	10.581	27.967	1.00	57.42	B
6992	CG	LYS	B1426	32.224	10.448	26.567	1.00	58.48	B
6993	CD	LYS	B1426	33.755	10.475	26.591	1.00	54.95	B
6994	CE	LYS	B1426	34.151	9.082	27.067	1.00	58.49	B
6995	NZ	LYS	B1426	35.524	8.561	26.782	1.00	52.36	B
6996	C	LYS	B1426	30.069	12.420	27.648	1.00	55.54	B
6997	O	LYS	B1426	29.824	12.679	26.488	1.00	56.10	B
6998	N	ASP	B1427	30.227	13.303	28.660	1.00	56.66	B
6999	CA	ASP	B1427	29.831	14.748	28.713	1.00	54.60	B
7000	CB	ASP	B1427	29.416	15.193	30.121	1.00	55.09	B
7001	CG	ASP	B1427	30.202	14.485	31.298	1.00	60.79	B
7002	OD1	ASP	B1427	31.334	13.991	31.053	1.00	55.73	B
7003	OD2	ASP	B1427	29.681	14.482	32.522	1.00	66.55	B
7004	C	ASP	B1427	31.062	15.367	28.265	1.00	53.44	B
7005	O	ASP	B1427	31.925	14.574	27.963	1.00	51.53	B
7006	N	SER	B1428	31.222	16.722	28.188	1.00	55.94	B
7007	CA	SER	B1428	32.669	17.372	28.036	1.00	56.51	B
7008	CB	SER	B1428	32.675	18.914	28.194	1.00	56.61	B
7009	OG	SER	B1428	31.395	19.542	28.403	1.00	61.75	B
7010	C	SER	B1428	33.908	16.786	28.891	1.00	55.62	B
7011	O	SER	B1428	35.037	16.682	28.439	1.00	54.04	B
7012	N	THR	B1429	33.684	16.398	30.127	1.00	55.98	B
7013	CA	THR	B1429	34.863	16.045	30.977	1.00	56.86	B
7014	CB	THR	B1429	34.624	16.193	32.506	1.00	56.94	B
7015	OG1	THR	B1429	34.254	14.878	33.021	1.00	61.29	B
7016	CG2	THR	B1429	33.515	17.338	32.888	1.00	50.41	B
7017	C	THR	B1429	35.341	14.599	30.743	1.00	57.82	B
7018	O	THR	B1429	36.540	14.300	31.015	1.00	59.41	B
7019	N	GLY	B1430	34.480	13.709	30.218	1.00	56.95	B
7020	CA	GLY	B1430	34.960	12.285	29.988	1.00	56.60	B
7021	C	GLY	B1430	34.346	11.212	30.896	1.00	56.20	B
7022	O	GLY	B1430	34.855	10.112	30.956	1.00	54.88	B
7023	N	LYS	B1431	33.256	11.530	31.597	1.00	55.31	B
7024	CA	LYS	B1431	32.537	10.455	32.265	1.00	59.41	B
7025	CB	LYS	B1431	31.971	10.810	33.717	1.00	60.00	B
7026	CG	LYS	B1431	32.601	11.990	34.576	1.00	63.56	B
7027	CD	LYS	B1431	31.610	13.396	34.614	1.00	66.10	B
7028	CE	LYS	B1431	31.985	14.550	35.704	1.00	62.32	B
7029	NZ	LYS	B1431	33.515	14.769	35.988	1.00	61.01	B
7030	C	LYS	B1431	31.427	9.687	31.341	1.00	59.25	B
7031	O	LYS	B1431	30.752	10.293	30.514	1.00	57.95	B
7032	N	TYR	B1432	31.264	8.367	31.571	1.00	57.70	B
7033	CA	TYR	B1432	30.506	7.457	30.735	1.00	56.10	B
7034	CB	TYR	B1432	31.137	6.068	30.756	1.00	54.71	B
7035	CG	TYR	B1432	31.951	5.930	29.487	1.00	56.73	B
7036	CD1	TYR	B1432	31.319	6.159	28.188	1.00	51.09	B
7037	CE1	TYR	B1432	32.122	6.073	26.947	1.00	56.13	B
7038	CD2	TYR	B1432	33.334	5.625	29.529	1.00	51.99	B
7039	CE2	TYR	B1432	34.122	5.599	28.268	1.00	58.49	B
7040	CZ	TYR	B1432	33.519	5.837	26.997	1.00	56.05	B
7041	OH	TYR	B1432	34.237	5.746	25.821	1.00	54.45	B
7042	C	TYR	B1432	29.175	7.425	31.314	1.00	55.69	B
7043	O	TYR	B1432	29.078	7.522	32.582	1.00	59.09	B

7044	N	TRP	B1433	28.116	7.448	30.479	1.00	53.45	B
7045	CA	TRP	B1433	26.751	7.414	31.052	1.00	51.73	B
7046	CB	TRP	B1433	25.679	7.283	29.965	1.00	49.10	B
7047	CG	TRP	B1433	25.346	8.639	29.381	1.00	53.31	B
7048	CD2	TRP	B1433	24.154	9.000	28.708	1.00	43.23	B
7049	CE2	TRP	B1433	24.245	10.373	28.411	1.00	47.22	B
7050	CE3	TRP	B1433	22.983	8.349	28.477	1.00	38.46	B
7051	CD1	TRP	B1433	26.200	9.788	29.279	1.00	52.73	B
7052	NE1	TRP	B1433	25.511	10.809	28.719	1.00	43.22	B
7053	CZ2	TRP	B1433	23.139	11.104	27.880	1.00	45.57	B
7054	CZ3	TRP	B1433	21.977	8.999	27.991	1.00	44.46	B
7055	CH2	TRP	B1433	22.026	10.418	27.705	1.00	45.14	B
7056	C	TRP	B1433	26.905	6.168	31.980	1.00	51.87	B
7057	O	TRP	B1433	27.451	5.078	31.517	1.00	50.68	B
7058	N	THR	B1434	26.535	6.362	33.250	1.00	51.13	B
7059	CA	THR	B1434	26.401	5.262	34.206	1.00	51.35	B
7060	CB	THR	B1434	27.175	5.403	35.647	1.00	52.30	B
7061	OG1	THR	B1434	27.354	6.778	36.159	1.00	41.93	B
7062	CG2	THR	B1434	28.197	4.353	35.876	1.00	48.37	B
7063	C	THR	B1434	25.113	5.411	34.935	1.00	54.04	B
7064	O	THR	B1434	24.817	6.609	35.425	1.00	52.57	B
7065	N	VAL	B1435	24.523	4.207	35.226	1.00	52.29	B
7066	CA	VAL	B1435	23.392	4.151	36.110	1.00	51.88	B
7067	CB	VAL	B1435	22.407	3.264	35.486	1.00	51.40	B
7068	CG1	VAL	B1435	22.902	2.981	34.149	1.00	44.26	B
7069	CG2	VAL	B1435	22.226	1.984	36.316	1.00	51.63	B
7070	C	VAL	B1435	23.564	3.821	37.620	1.00	54.42	B
7071	O	VAL	B1435	24.469	3.088	37.990	1.00	55.82	B
7072	N	GLY	B1436	22.621	4.294	38.484	1.00	55.72	B
7073	CA	GLY	B1436	22.620	4.068	39.945	1.00	53.69	B
7074	C	GLY	B1436	21.741	2.930	40.548	1.00	54.20	B
7075	O	GLY	B1436	21.355	1.970	39.850	1.00	50.59	B
7076	N	SER	B1437	21.442	3.066	41.884	1.00	54.80	B
7077	CA	SER	B1437	20.843	2.030	42.737	1.00	53.74	B
7078	CB	SER	B1437	21.416	2.120	44.185	1.00	54.61	B
7079	OG	SER	B1437	20.465	1.895	45.258	1.00	48.21	B
7080	C	SER	B1437	19.331	2.197	42.614	1.00	55.58	B
7081	O	SER	B1437	18.586	1.240	42.945	1.00	56.99	B
7082	N	ASP	B1438	18.895	3.392	42.148	1.00	55.66	B
7083	CA	ASP	B1438	17.544	3.671	41.508	1.00	56.46	B
7084	CB	ASP	B1438	17.039	4.972	42.106	1.00	56.26	B
7085	CG	ASP	B1438	18.080	6.069	41.974	1.00	63.81	B
7086	OD1	ASP	B1438	18.316	6.650	40.863	1.00	63.50	B
7087	OD2	ASP	B1438	18.730	6.295	43.035	1.00	78.35	B
7088	C	ASP	B1438	17.666	4.031	40.020	1.00	54.34	B
7089	O	ASP	B1438	17.505	5.220	39.670	1.00	55.87	B
7090	N	SER	B1439	18.060	3.115	39.177	1.00	51.07	B
7091	CA	SER	B1439	18.138	3.382	37.752	1.00	51.63	B
7092	CB	SER	B1439	16.871	2.838	37.088	1.00	51.33	B
7093	OG	SER	B1439	16.234	2.007	38.049	1.00	56.65	B
7094	C	SER	B1439	18.400	4.905	37.265	1.00	51.97	B
7095	O	SER	B1439	18.406	5.203	35.993	1.00	49.08	B
7096	N	ALA	B1440	18.635	5.805	38.259	1.00	50.17	B
7097	CA	ALA	B1440	19.263	7.123	37.925	1.00	51.83	B
7098	CB	ALA	B1440	19.880	7.940	39.256	1.00	48.64	B
7099	C	ALA	B1440	20.301	6.966	36.755	1.00	51.32	B

7100	O	ALA	B1440	20.828	5.855	36.593	1.00	52.84	B
7101	N	VAL	B1441	20.529	7.966	35.900	1.00	49.82	B
7102	CA	VAL	B1441	21.621	7.793	34.910	1.00	47.95	B
7103	CB	VAL	B1441	21.256	7.717	33.296	1.00	48.83	B
7104	CG1	VAL	B1441	22.484	7.663	32.420	1.00	45.67	B
7105	CG2	VAL	B1441	20.368	6.562	32.774	1.00	43.37	B
7106	C	VAL	B1441	22.396	9.073	35.101	1.00	47.96	B
7107	O	VAL	B1441	21.807	10.136	35.301	1.00	45.86	B
7108	N	THR	B1442	23.738	8.950	35.003	1.00	47.45	B
7109	CA	THR	B1442	24.623	10.003	35.151	1.00	45.49	B
7110	CB	THR	B1442	24.921	10.251	36.705	1.00	43.52	B
7111	OG1	THR	B1442	25.305	9.036	37.250	1.00	47.75	B
7112	CG2	THR	B1442	23.673	10.585	37.488	1.00	38.83	B
7113	C	THR	B1442	25.851	9.648	34.258	1.00	48.81	B
7114	O	THR	B1442	26.187	8.431	33.936	1.00	44.75	B
7115	N	SER	B1443	26.537	10.718	33.860	1.00	52.00	B
7116	CA	SER	B1443	27.572	10.500	32.897	1.00	58.20	B
7117	CB	SER	B1443	27.615	11.711	31.894	1.00	59.21	B
7118	OG	SER	B1443	28.299	11.352	30.685	1.00	63.08	B
7119	C	SER	B1443	28.835	10.475	33.722	1.00	60.92	B
7120	O	SER	B1443	29.943	10.207	33.225	1.00	59.33	B
7121	N	SER	B1444	28.624	10.948	34.959	1.00	64.82	B
7122	CA	SER	B1444	29.494	10.799	36.121	1.00	67.47	B
7123	CB	SER	B1444	28.657	11.196	37.397	1.00	69.94	B
7124	OG	SER	B1444	28.338	12.649	37.469	1.00	72.73	B
7125	C	SER	B1444	29.887	9.319	36.066	1.00	68.45	B
7126	O	SER	B1444	29.134	8.472	35.489	1.00	69.57	B
7127	N	GLY	B1445	31.111	9.002	36.506	1.00	69.09	B
7128	CA	GLY	B1445	31.600	7.608	36.481	1.00	67.75	B
7129	C	GLY	B1445	32.336	7.276	35.248	1.00	67.55	B
7130	O	GLY	B1445	31.914	6.539	34.403	1.00	67.31	B
7131	N	ASP	B1446	33.505	7.852	35.173	1.00	68.15	B
7132	CA	ASP	B1446	34.514	7.465	34.183	1.00	67.39	B
7133	CB	ASP	B1446	35.833	8.286	34.493	1.00	66.62	B
7134	CG	ASP	B1446	35.628	9.907	34.500	1.00	61.40	B
7135	OD1	ASP	B1446	36.676	10.616	34.390	1.00	48.79	B
7136	OD2	ASP	B1446	34.451	10.421	34.553	1.00	49.99	B
7137	C	ASP	B1446	34.761	5.901	34.108	1.00	68.59	B
7138	O	ASP	B1446	35.757	5.377	34.767	1.00	67.10	B
7139	N	THR	B1447	33.878	5.209	33.310	1.00	68.95	B
7140	CA	THR	B1447	33.720	3.661	33.194	1.00	69.23	B
7141	CB	THR	B1447	33.329	3.031	34.639	1.00	70.85	B
7142	OG1	THR	B1447	34.142	3.611	35.712	1.00	70.45	B
7143	CG2	THR	B1447	33.319	1.457	34.662	1.00	69.40	B
7144	C	THR	B1447	32.728	3.049	32.023	1.00	69.56	B
7145	O	THR	B1447	31.474	3.289	31.990	1.00	67.02	B
7146	N	PRO	B1448	33.298	2.330	31.015	1.00	68.73	B
7147	CD	PRO	B1448	34.723	1.950	30.855	1.00	69.37	B
7148	CA	PRO	B1448	32.495	1.969	29.815	1.00	67.70	B
7149	CB	PRO	B1448	33.535	1.275	28.872	1.00	68.21	B
7150	CG	PRO	B1448	34.915	1.779	29.335	1.00	66.71	B
7151	C	PRO	B1448	31.325	1.007	30.065	1.00	66.91	B
7152	O	PRO	B1448	31.553	-0.276	30.241	1.00	65.10	B
7153	N	VAL	B1449	30.086	1.591	30.055	1.00	64.63	B
7154	CA	VAL	B1449	28.808	0.778	29.909	1.00	60.31	B
7155	CB	VAL	B1449	27.826	1.071	31.064	1.00	60.49	B

7156	CG1	VAL	B1449	28.162	0.265	32.178	1.00	59.14	B
7157	CG2	VAL	B1449	27.758	2.572	31.413	1.00	56.18	B
7158	C	VAL	B1449	28.107	0.829	28.479	1.00	60.46	B
7159	O	VAL	B1449	28.409	1.685	27.717	1.00	61.94	B
7160	N	ASP	B1450	27.166	-0.056	28.143	1.00	59.32	B
7161	CA	ASP	B1450	26.606	-0.218	26.764	1.00	56.26	B
7162	CB	ASP	B1450	26.756	-1.679	26.203	1.00	54.81	B
7163	CG	ASP	B1450	28.135	-1.928	25.685	1.00	60.05	B
7164	OD1	ASP	B1450	28.580	-3.058	25.283	1.00	58.35	B
7165	OD2	ASP	B1450	28.815	-0.881	25.729	1.00	66.19	B
7166	C	ASP	B1450	25.159	0.140	26.723	1.00	53.17	B
7167	O	ASP	B1450	24.226	-0.658	27.061	1.00	51.38	B
7168	N	PHE	B1451	24.870	1.268	26.133	1.00	51.88	B
7169	CA	PHE	B1451	23.462	1.416	25.928	1.00	49.79	B
7170	CB	PHE	B1451	23.057	2.799	26.015	1.00	49.88	B
7171	CG	PHE	B1451	23.443	3.492	27.336	1.00	48.88	B
7172	CD1	PHE	B1451	24.755	3.494	27.806	1.00	48.02	B
7173	CD2	PHE	B1451	22.532	4.222	28.013	1.00	49.64	B
7174	CE1	PHE	B1451	25.098	4.179	28.866	1.00	47.05	B
7175	CE2	PHE	B1451	22.897	4.875	29.176	1.00	52.47	B
7176	CZ	PHE	B1451	24.174	4.899	29.572	1.00	47.93	B
7177	C	PHE	B1451	23.129	0.853	24.629	1.00	51.05	B
7178	O	PHE	B1451	24.070	0.520	23.780	1.00	49.64	B
7179	N	PHE	B1452	21.807	0.645	24.491	1.00	53.19	B
7180	CA	PHE	B1452	21.190	0.059	23.244	1.00	56.62	B
7181	CB	PHE	B1452	20.516	-1.294	23.538	1.00	57.59	B
7182	CG	PHE	B1452	21.520	-2.280	23.978	1.00	59.48	B
7183	CD1	PHE	B1452	22.300	-2.021	25.192	1.00	60.99	B
7184	CD2	PHE	B1452	21.913	-3.263	23.107	1.00	58.76	B
7185	CE1	PHE	B1452	23.359	-2.844	25.604	1.00	57.95	B
7186	CE2	PHE	B1452	22.923	-4.097	23.490	1.00	65.31	B
7187	CZ	PHE	B1452	23.666	-3.892	24.796	1.00	62.58	B
7188	C	PHE	B1452	20.259	0.997	22.702	1.00	57.06	B
7189	O	PHE	B1452	19.419	1.415	23.471	1.00	63.15	B
7190	N	PHE	B1453	20.426	1.436	21.471	1.00	54.98	B
7191	CA	PHE	B1453	19.463	2.351	20.845	1.00	52.18	B
7192	CB	PHE	B1453	20.182	3.268	19.846	1.00	54.43	B
7193	CG	PHE	B1453	20.811	4.410	20.453	1.00	53.97	B
7194	CD1	PHE	B1453	20.687	4.633	21.787	1.00	54.57	B
7195	CD2	PHE	B1453	21.625	5.188	19.706	1.00	51.78	B
7196	CE1	PHE	B1453	21.391	5.733	22.351	1.00	58.98	B
7197	CE2	PHE	B1453	22.307	6.234	20.233	1.00	51.46	B
7198	CZ	PHE	B1453	22.226	6.536	21.532	1.00	52.10	B
7199	C	PHE	B1453	18.518	1.630	19.909	1.00	50.52	B
7200	O	PHE	B1453	18.940	0.821	19.155	1.00	49.02	B
7201	N	GLU	B1454	17.268	2.049	19.841	1.00	51.26	B
7202	CA	GLU	B1454	16.192	1.387	19.036	1.00	50.28	B
7203	CB	GLU	B1454	15.150	0.791	19.970	1.00	49.69	B
7204	CG	GLU	B1454	15.863	-0.129	21.040	1.00	50.67	B
7205	CD	GLU	B1454	15.058	-1.251	21.610	1.00	55.45	B
7206	OE1	GLU	B1454	15.791	-2.145	22.157	1.00	53.20	B
7207	OE2	GLU	B1454	13.766	-1.292	21.443	1.00	53.30	B
7208	C	GLU	B1454	15.650	2.532	18.314	1.00	50.70	B
7209	O	GLU	B1454	15.437	3.604	18.988	1.00	51.25	B
7210	N	PHE	B1455	15.614	2.448	16.950	1.00	50.53	B
7211	CA	PHE	B1455	15.011	3.554	16.155	1.00	48.49	B

7212	CB	PHE	B1455	15.750	3.934	15.010	1.00	45.46	B
7213	CG	PHE	B1455	17.170	4.315	15.233	1.00	44.30	B
7214	CD1	PHE	B1455	18.221	3.300	15.221	1.00	48.56	B
7215	CD2	PHE	B1455	17.531	5.671	15.305	1.00	42.67	B
7216	CE1	PHE	B1455	19.567	3.623	15.343	1.00	43.12	B
7217	CE2	PHE	B1455	18.878	6.100	15.464	1.00	36.47	B
7218	CZ	PHE	B1455	19.916	5.067	15.484	1.00	45.39	B
7219	C	PHE	B1455	13.558	3.239	15.753	1.00	52.06	B
7220	O	PHE	B1455	13.216	2.601	14.741	1.00	54.58	B
7221	N	CYS	B1456	12.714	3.748	16.610	1.00	53.29	B
7222	CA	CYS	B1456	11.388	3.458	16.802	1.00	54.89	B
7223	CB	CYS	B1456	11.281	3.676	18.348	1.00	55.17	B
7224	SG	CYS	B1456	11.848	2.277	18.972	1.00	62.12	B
7225	C	CYS	B1456	10.543	4.481	16.132	1.00	55.04	B
7226	O	CYS	B1456	9.291	4.373	16.109	1.00	55.69	B
7227	N	ASP	B1457	11.156	5.558	15.723	1.00	55.08	B
7228	CA	ASP	B1457	10.363	6.476	15.059	1.00	58.38	B
7229	CB	ASP	B1457	10.037	7.603	15.964	1.00	60.77	B
7230	CG	ASP	B1457	9.128	7.225	17.032	1.00	66.77	B
7231	OD1	ASP	B1457	7.900	7.675	16.832	1.00	71.86	B
7232	OD2	ASP	B1457	9.641	6.465	17.990	1.00	61.07	B
7233	C	ASP	B1457	11.298	7.090	14.138	1.00	60.45	B
7234	O	ASP	B1457	12.555	6.904	14.270	1.00	59.46	B
7235	N	TYR	B1458	10.675	7.966	13.307	1.00	61.25	B
7236	CA	TYR	B1458	11.306	8.412	12.065	1.00	61.52	B
7237	CB	TYR	B1458	10.347	9.024	11.052	1.00	61.41	B
7238	CG	TYR	B1458	9.634	10.136	11.649	1.00	66.46	B
7239	CD1	TYR	B1458	10.034	11.463	11.356	1.00	67.99	B
7240	CE1	TYR	B1458	9.419	12.529	11.988	1.00	71.01	B
7241	CD2	TYR	B1458	8.601	9.894	12.587	1.00	66.33	B
7242	CE2	TYR	B1458	7.943	10.960	13.196	1.00	70.64	B
7243	CZ	TYR	B1458	8.376	12.287	12.904	1.00	69.78	B
7244	OH	TYR	B1458	7.745	13.386	13.472	1.00	70.03	B
7245	C	TYR	B1458	12.301	9.377	12.489	1.00	59.69	B
7246	O	TYR	B1458	13.240	9.604	11.787	1.00	60.39	B
7247	N	ASN	B1459	12.122	9.947	13.656	1.00	56.36	B
7248	CA	ASN	B1459	13.167	10.821	13.991	1.00	55.87	B
7249	CB	ASN	B1459	12.782	12.258	13.648	1.00	55.60	B
7250	CG	ASN	B1459	11.607	12.690	14.435	1.00	56.33	B
7251	OD1	ASN	B1459	10.799	11.861	14.907	1.00	58.79	B
7252	ND2	ASN	B1459	11.420	13.979	14.509	1.00	54.32	B
7253	C	ASN	B1459	13.710	10.593	15.412	1.00	53.48	B
7254	O	ASN	B1459	14.746	11.128	15.698	1.00	52.72	B
7255	N	LYS	B1460	13.086	9.664	16.132	1.00	51.45	B
7256	CA	LYS	B1460	13.393	9.303	17.462	1.00	51.74	B
7257	CB	LYS	B1460	12.133	9.249	18.370	1.00	51.60	B
7258	CG	LYS	B1460	11.194	10.519	18.585	1.00	55.18	B
7259	CD	LYS	B1460	9.788	10.371	17.906	1.00	55.95	B
7260	CE	LYS	B1460	8.819	11.516	18.181	1.00	52.32	B
7261	NZ	LYS	B1460	7.272	11.181	17.989	1.00	48.55	B
7262	C	LYS	B1460	14.057	7.942	17.645	1.00	53.06	B
7263	O	LYS	B1460	13.865	6.946	16.810	1.00	53.05	B
7264	N	VAL	B1461	14.680	7.829	18.846	1.00	51.75	B
7265	CA	VAL	B1461	15.409	6.659	19.217	1.00	49.19	B
7266	CB	VAL	B1461	16.834	6.994	19.078	1.00	49.92	B
7267	CG1	VAL	B1461	17.325	7.899	20.199	1.00	42.55	B

7268	CG2	VAL	B1461	17.741	5.706	18.753	1.00	50.60	B
7269	C	VAL	B1461	15.095	6.478	20.664	1.00	50.75	B
7270	O	VAL	B1461	14.927	7.418	21.399	1.00	52.10	B
7271	N	ALA	B1462	14.972	5.246	21.099	1.00	50.56	B
7272	CA	ALA	B1462	14.698	4.954	22.449	1.00	48.87	B
7273	CB	ALA	B1462	13.565	4.056	22.505	1.00	46.24	B
7274	C	ALA	B1462	16.034	4.345	23.058	1.00	49.38	B
7275	O	ALA	B1462	16.922	3.872	22.312	1.00	50.01	B
7276	N	ILE	B1463	16.222	4.388	24.363	1.00	47.94	B
7277	CA	ILE	B1463	17.551	4.025	24.835	1.00	47.11	B
7278	CB	ILE	B1463	18.344	5.225	25.292	1.00	48.94	B
7279	CG2	ILE	B1463	19.869	4.727	25.698	1.00	46.52	B
7280	CG1	ILE	B1463	18.143	6.423	24.269	1.00	51.05	B
7281	CD1	ILE	B1463	18.669	7.792	24.570	1.00	44.98	B
7282	C	ILE	B1463	17.500	3.107	26.002	1.00	49.20	B
7283	O	ILE	B1463	17.120	3.510	27.239	1.00	46.01	B
7284	N	LYS	B1464	17.890	1.880	25.616	1.00	50.69	B
7285	CA	LYS	B1464	17.625	0.582	26.446	1.00	53.41	B
7286	CB	LYS	B1464	17.322	-0.632	25.633	1.00	51.69	B
7287	CG	LYS	B1464	16.964	-1.783	26.441	1.00	58.03	B
7288	CD	LYS	B1464	17.777	-3.136	26.086	1.00	62.97	B
7289	CE	LYS	B1464	17.049	-4.179	25.146	1.00	49.51	B
7290	NZ	LYS	B1464	16.141	-4.963	25.999	1.00	49.33	B
7291	C	LYS	B1464	18.905	0.355	27.147	1.00	53.63	B
7292	O	LYS	B1464	19.927	0.572	26.466	1.00	53.71	B
7293	N	VAL	B1465	18.808	0.142	28.475	1.00	53.24	B
7294	CA	VAL	B1465	19.932	-0.245	29.412	1.00	54.84	B
7295	CB	VAL	B1465	21.052	0.860	29.725	1.00	55.07	B
7296	CG1	VAL	B1465	20.459	2.135	30.238	1.00	58.21	B
7297	CG2	VAL	B1465	22.193	0.400	30.639	1.00	49.92	B
7298	C	VAL	B1465	19.322	-0.918	30.632	1.00	54.16	B
7299	O	VAL	B1465	18.307	-0.502	31.116	1.00	53.64	B
7300	N	GLY	B1466	19.862	-2.088	30.952	1.00	54.33	B
7301	CA	GLY	B1466	19.346	-2.975	32.018	1.00	51.98	B
7302	C	GLY	B1466	17.987	-3.236	31.515	1.00	50.81	B
7303	O	GLY	B1466	17.138	-2.892	32.151	1.00	54.12	B
7304	N	GLY	B1467	17.741	-3.859	30.392	1.00	49.31	B
7305	CA	GLY	B1467	16.405	-4.170	30.013	1.00	47.50	B
7306	C	GLY	B1467	15.390	-3.147	30.417	1.00	50.17	B
7307	O	GLY	B1467	14.223	-3.503	30.576	1.00	51.96	B
7308	N	ARG	B1468	15.739	-1.903	30.736	1.00	51.17	B
7309	CA	ARG	B1468	14.666	-0.768	30.691	1.00	54.30	B
7310	CB	ARG	B1468	14.583	-0.132	32.061	1.00	51.82	B
7311	CG	ARG	B1468	13.899	-0.835	32.861	1.00	53.87	B
7312	CD	ARG	B1468	14.857	-1.336	34.022	1.00	66.93	B
7313	NE	ARG	B1468	13.958	-2.097	34.957	1.00	70.69	B
7314	CZ	ARG	B1468	14.272	-2.895	35.958	1.00	64.02	B
7315	NH1	ARG	B1468	15.529	-3.133	36.239	1.00	62.58	B
7316	NH2	ARG	B1468	13.268	-3.479	36.606	1.00	62.52	B
7317	C	ARG	B1468	14.843	0.434	29.545	1.00	55.81	B
7318	O	ARG	B1468	15.751	0.350	28.618	1.00	57.93	B
7319	N	TYR	B1469	14.177	1.592	29.703	1.00	54.91	B
7320	CA	TYR	B1469	14.512	2.722	28.806	1.00	54.21	B
7321	CB	TYR	B1469	13.377	3.012	27.695	1.00	52.56	B
7322	CG	TYR	B1469	13.315	1.875	26.689	1.00	51.66	B
7323	CD1	TYR	B1469	14.149	1.792	25.555	1.00	51.12	B

7324	CE1	TYR	B1469	13.983	0.560	24.597	1.00	50.58	B
7325	CD2	TYR	B1469	12.443	0.786	26.928	1.00	56.88	B
7326	CE2	TYR	B1469	12.345	-0.340	26.108	1.00	54.54	B
7327	CZ	TYR	B1469	13.127	-0.461	24.956	1.00	54.25	B
7328	OH	TYR	B1469	12.967	-1.665	24.335	1.00	49.99	B
7329	C	TYR	B1469	14.901	3.932	29.546	1.00	53.37	B
7330	O	TYR	B1469	14.385	4.190	30.548	1.00	53.21	B
7331	N	LEU	B1470	15.772	4.728	29.002	1.00	54.95	B
7332	CA	LEU	B1470	15.991	5.994	29.638	1.00	58.05	B
7333	CB	LEU	B1470	16.987	6.836	28.852	1.00	58.93	B
7334	CG	LEU	B1470	18.469	7.020	29.233	1.00	61.91	B
7335	CD1	LEU	B1470	19.294	5.771	29.093	1.00	60.88	B
7336	CD2	LEU	B1470	19.060	8.081	28.373	1.00	59.27	B
7337	C	LEU	B1470	14.774	6.751	29.463	1.00	58.65	B
7338	O	LEU	B1470	14.487	6.984	28.348	1.00	59.27	B
7339	N	LYS	B1471	14.116	7.172	30.576	1.00	60.28	B
7340	CA	LYS	B1471	12.914	8.058	30.640	1.00	59.74	B
7341	CB	LYS	B1471	11.674	7.155	30.853	1.00	57.21	B
7342	CG	LYS	B1471	10.375	7.885	30.803	1.00	55.54	B
7343	CD	LYS	B1471	9.354	7.011	31.569	1.00	56.04	B
7344	CE	LYS	B1471	7.898	7.643	31.856	1.00	46.04	B
7345	NZ	LYS	B1471	6.787	6.672	32.531	1.00	46.36	B
7346	C	LYS	B1471	12.981	9.178	31.799	1.00	61.35	B
7347	O	LYS	B1471	12.898	8.814	33.045	1.00	60.16	B
7348	N	GLY	B1472	13.113	10.491	31.399	1.00	61.22	B
7349	CA	GLY	B1472	13.028	11.632	32.330	1.00	62.05	B
7350	C	GLY	B1472	11.801	11.644	33.239	1.00	64.71	B
7351	O	GLY	B1472	10.750	11.989	32.711	1.00	70.04	B
7352	N	ASP	B1473	11.874	11.301	34.548	1.00	63.13	B
7353	CA	ASP	B1473	10.765	11.264	35.565	1.00	62.42	B
7354	CB	ASP	B1473	11.220	10.377	36.711	1.00	61.90	B
7355	CG	ASP	B1473	12.035	11.154	37.782	1.00	64.29	B
7356	OD1	ASP	B1473	13.099	11.766	37.455	1.00	66.79	B
7357	OD2	ASP	B1473	11.604	11.138	38.974	1.00	57.99	B
7358	C	ASP	B1473	10.164	12.558	36.256	1.00	62.63	B
7359	O	ASP	B1473	10.329	13.654	35.751	1.00	63.67	B
7360	N	HIS	B1474	9.400	12.409	37.359	1.00	62.29	B
7361	CA	HIS	B1474	9.087	13.550	38.288	1.00	63.94	B
7362	CB	HIS	B1474	8.653	13.038	39.683	1.00	64.81	B
7363	CG	HIS	B1474	7.566	12.006	39.661	1.00	68.36	B
7364	CD2	HIS	B1474	6.363	11.962	40.312	1.00	64.57	B
7365	ND1	HIS	B1474	7.659	10.826	38.913	1.00	70.49	B
7366	CE1	HIS	B1474	6.541	10.132	39.076	1.00	70.06	B
7367	NE2	HIS	B1474	5.737	10.804	39.909	1.00	63.39	B
7368	C	HIS	B1474	10.333	14.505	38.530	1.00	64.13	B
7369	O	HIS	B1474	11.478	14.048	38.832	1.00	61.98	B
7370	N	ALA	B1475	10.109	15.821	38.367	1.00	64.45	B
7371	CA	ALA	B1475	11.246	16.874	38.315	1.00	63.45	B
7372	CB	ALA	B1475	11.968	17.016	39.671	1.00	62.92	B
7373	C	ALA	B1475	12.278	16.731	37.157	1.00	62.14	B
7374	O	ALA	B1475	13.073	17.695	36.962	1.00	62.08	B
7375	N	GLY	B1476	12.267	15.586	36.404	1.00	59.08	B
7376	CA	GLY	B1476	12.982	15.489	35.146	1.00	57.91	B
7377	C	GLY	B1476	14.178	14.578	35.116	1.00	59.13	B
7378	O	GLY	B1476	14.966	14.606	34.199	1.00	60.45	B
7379	N	VAL	B1477	14.323	13.683	36.068	1.00	59.24	B

7380	CA	VAL	B1477	15.606	13.027	36.203	1.00	57.80	B
7381	CB	VAL	B1477	15.758	12.467	37.589	1.00	58.76	B
7382	CG1	VAL	B1477	16.975	11.321	37.735	1.00	56.85	B
7383	CG2	VAL	B1477	15.866	13.655	38.516	1.00	57.94	B
7384	C	VAL	B1477	15.709	11.945	35.253	1.00	56.77	B
7385	O	VAL	B1477	14.840	11.112	35.224	1.00	57.22	B
7386	N	LEU	B1478	16.800	11.866	34.526	1.00	55.22	B
7387	CA	LEU	B1478	16.884	10.737	33.638	1.00	55.04	B
7388	CB	LEU	B1478	17.985	10.978	32.674	1.00	55.44	B
7389	CG	LEU	B1478	17.857	10.187	31.391	1.00	56.59	B
7390	CD1	LEU	B1478	16.575	10.635	30.734	1.00	49.56	B
7391	CD2	LEU	B1478	19.142	10.522	30.554	1.00	52.63	B
7392	C	LEU	B1478	16.995	9.329	34.282	1.00	55.91	B
7393	O	LEU	B1478	18.103	8.920	34.705	1.00	58.31	B
7394	N	LYS	B1479	15.875	8.609	34.431	1.00	53.49	B
7395	CA	LYS	B1479	16.015	7.293	34.954	1.00	53.36	B
7396	CB	LYS	B1479	15.176	7.097	36.173	1.00	52.59	B
7397	CG	LYS	B1479	14.982	8.364	37.052	1.00	54.99	B
7398	CD	LYS	B1479	14.537	8.040	38.497	1.00	49.56	B
7399	CE	LYS	B1479	15.504	8.442	39.496	1.00	46.63	B
7400	NZ	LYS	B1479	15.587	7.438	40.576	1.00	46.04	B
7401	C	LYS	B1479	15.707	6.264	33.862	1.00	55.21	B
7402	O	LYS	B1479	14.907	6.515	32.895	1.00	57.50	B
7403	N	ALA	B1480	16.333	5.102	34.000	1.00	53.43	B
7404	CA	ALA	B1480	16.122	4.022	33.067	1.00	53.10	B
7405	CB	ALA	B1480	17.372	3.249	32.933	1.00	53.64	B
7406	C	ALA	B1480	15.142	3.080	33.589	1.00	52.82	B
7407	O	ALA	B1480	15.537	2.065	33.992	1.00	55.98	B
7408	N	SER	B1481	13.874	3.369	33.568	1.00	53.48	B
7409	CA	SER	B1481	12.863	2.566	34.242	1.00	55.45	B
7410	CB	SER	B1481	12.401	3.322	35.488	1.00	55.69	B
7411	OG	SER	B1481	11.961	4.646	35.003	1.00	58.38	B
7412	C	SER	B1481	11.634	2.352	33.358	1.00	56.84	B
7413	O	SER	B1481	10.879	1.425	33.662	1.00	59.65	B
7414	N	ALA	B1482	11.431	3.141	32.294	1.00	56.64	B
7415	CA	ALA	B1482	10.315	2.949	31.345	1.00	59.13	B
7416	CB	ALA	B1482	10.544	3.706	30.119	1.00	59.98	B
7417	C	ALA	B1482	10.138	1.559	30.907	1.00	60.45	B
7418	O	ALA	B1482	11.188	0.940	30.594	1.00	62.40	B
7419	N	GLU	B1483	8.894	1.030	30.788	1.00	60.61	B
7420	CA	GLU	B1483	8.944	-0.461	30.655	1.00	63.29	B
7421	CB	GLU	B1483	7.883	-1.333	31.341	1.00	63.32	B
7422	CG	GLU	B1483	8.296	-2.942	31.247	1.00	59.35	B
7423	CD	GLU	B1483	9.265	-3.240	32.425	1.00	57.98	B
7424	OE1	GLU	B1483	9.012	-3.927	33.413	1.00	60.33	B
7425	OE2	GLU	B1483	10.324	-2.684	32.419	1.00	57.13	B
7426	C	GLU	B1483	9.039	-0.927	29.270	1.00	63.19	B
7427	O	GLU	B1483	9.633	-2.019	28.985	1.00	62.34	B
7428	N	THR	B1484	8.427	-0.093	28.441	1.00	62.70	B
7429	CA	THR	B1484	8.303	-0.413	27.060	1.00	64.59	B
7430	CB	THR	B1484	6.990	-1.050	26.748	1.00	64.67	B
7431	OG1	THR	B1484	6.027	-0.587	27.708	1.00	68.57	B
7432	CG2	THR	B1484	7.093	-2.554	26.779	1.00	65.31	B
7433	C	THR	B1484	8.166	0.868	26.385	1.00	65.19	B
7434	O	THR	B1484	7.122	1.573	26.587	1.00	67.95	B
7435	N	VAL	B1485	9.171	1.177	25.549	1.00	63.27	B

7436	CA	VAL	B1485	9.001	2.201	24.522	1.00	58.53	B
7437	CB	VAL	B1485	8.940	1.607	23.173	1.00	57.24	B
7438	CG1	VAL	B1485	9.851	2.377	22.386	1.00	57.26	B
7439	CG2	VAL	B1485	9.230	-0.058	23.094	1.00	59.27	B
7440	C	VAL	B1485	7.774	3.132	24.675	1.00	58.07	B
7441	O	VAL	B1485	6.624	2.647	24.770	1.00	57.57	B
7442	N	ASP	B1486	7.960	4.454	24.694	1.00	56.23	B
7443	CA	ASP	B1486	6.737	5.288	24.507	1.00	55.55	B
7444	CB	ASP	B1486	5.883	5.277	25.806	1.00	57.79	B
7445	CG	ASP	B1486	6.697	5.809	27.107	1.00	55.70	B
7446	OD1	ASP	B1486	6.102	5.911	28.132	1.00	50.86	B
7447	OD2	ASP	B1486	7.920	6.065	27.055	1.00	55.56	B
7448	C	ASP	B1486	7.407	6.627	24.448	1.00	55.42	B
7449	O	ASP	B1486	8.681	6.576	24.633	1.00	54.87	B
7450	N	PRO	B1487	6.571	7.747	24.410	1.00	51.92	B
7451	CD	PRO	B1487	5.140	7.367	24.341	1.00	49.86	B
7452	CA	PRO	B1487	6.740	9.216	24.453	1.00	53.23	B
7453	CB	PRO	B1487	5.294	9.813	24.686	1.00	52.51	B
7454	CG	PRO	B1487	4.314	8.739	24.461	1.00	48.36	B
7455	C	PRO	B1487	7.682	9.800	25.502	1.00	53.98	B
7456	O	PRO	B1487	8.476	10.639	25.145	1.00	56.24	B
7457	N	ALA	B1488	7.617	9.329	26.742	1.00	53.47	B
7458	CA	ALA	B1488	8.621	9.654	27.775	1.00	53.83	B
7459	CB	ALA	B1488	8.128	9.080	29.214	1.00	51.24	B
7460	C	ALA	B1488	10.019	9.105	27.420	1.00	53.64	B
7461	O	ALA	B1488	10.910	9.806	27.180	1.00	54.12	B
7462	N	SER	B1489	10.173	7.805	27.397	1.00	55.24	B
7463	CA	SER	B1489	11.335	7.182	26.908	1.00	56.22	B
7464	CB	SER	B1489	11.475	5.744	27.412	1.00	54.99	B
7465	OG	SER	B1489	10.195	5.107	27.444	1.00	63.21	B
7466	C	SER	B1489	11.458	7.302	25.389	1.00	55.71	B
7467	O	SER	B1489	11.521	6.329	24.697	1.00	58.63	B
7468	N	LEU	B1490	11.519	8.510	24.869	1.00	55.54	B
7469	CA	LEU	B1490	12.016	8.712	23.490	1.00	53.60	B
7470	CB	LEU	B1490	10.921	8.502	22.514	1.00	53.36	B
7471	CG	LEU	B1490	10.431	7.352	21.697	1.00	51.34	B
7472	CD1	LEU	B1490	9.067	8.058	21.183	1.00	52.37	B
7473	CD2	LEU	B1490	11.383	7.075	20.480	1.00	51.94	B
7474	C	LEU	B1490	12.400	10.184	23.287	1.00	53.65	B
7475	O	LEU	B1490	11.915	11.100	24.076	1.00	51.62	B
7476	N	TRP	B1491	13.214	10.361	22.223	1.00	51.38	B
7477	CA	TRP	B1491	14.049	11.509	21.950	1.00	51.14	B
7478	CB	TRP	B1491	15.419	11.202	22.626	1.00	50.85	B
7479	CG	TRP	B1491	15.287	10.460	24.061	1.00	50.05	B
7480	CD2	TRP	B1491	14.865	11.084	25.382	1.00	50.02	B
7481	CE2	TRP	B1491	14.894	10.050	26.336	1.00	48.70	B
7482	CE3	TRP	B1491	14.539	12.422	25.823	1.00	47.12	B
7483	CD1	TRP	B1491	15.562	9.169	24.312	1.00	43.94	B
7484	NE1	TRP	B1491	15.319	8.912	25.647	1.00	49.67	B
7485	CZ2	TRP	B1491	14.580	10.273	27.724	1.00	44.77	B
7486	CZ3	TRP	B1491	14.160	12.635	27.262	1.00	46.30	B
7487	CH2	TRP	B1491	14.164	11.565	28.147	1.00	43.91	B
7488	C	TRP	B1491	14.378	11.678	20.425	1.00	51.92	B
7489	O	TRP	B1491	14.422	10.713	19.710	1.00	52.85	B
7490	N	GLU	B1492	14.667	12.887	20.006	1.00	50.46	B
7491	CA	GLU	B1492	15.290	13.190	18.799	1.00	51.35	B

7492	CB	GLU	B	1492	14.706	14.535	18.172	1.00	51.01	B
7493	CG	GLU	B	1492	13.121	14.587	18.104	1.00	50.74	B
7494	CD	GLU	B	1492	12.461	15.964	18.296	1.00	52.68	B
7495	OE1	GLU	B	1492	13.156	17.023	18.118	1.00	49.77	B
7496	OE2	GLU	B	1492	11.205	15.988	18.692	1.00	46.64	B
7497	C	GLU	B	1492	16.831	13.226	18.913	1.00	51.55	B
7498	O	GLU	B	1492	17.485	14.200	19.436	1.00	51.33	B
7499	N	TYR	B	1493	17.473	12.210	18.374	1.00	49.11	B
7500	CA	TYR	B	1493	18.896	12.433	18.069	1.00	47.50	B
7501	CB	TYR	B	1493	19.474	11.161	17.576	1.00	47.06	B
7502	CG	TYR	B	1493	18.712	10.498	16.487	1.00	45.62	B
7503	CD1	TYR	B	1493	17.524	9.814	16.761	1.00	51.35	B
7504	CE1	TYR	B	1493	16.831	9.135	15.745	1.00	51.24	B
7505	CD2	TYR	B	1493	19.217	10.467	15.182	1.00	43.39	B
7506	CE2	TYR	B	1493	18.601	9.788	14.193	1.00	39.85	B
7507	CZ	TYR	B	1493	17.430	9.130	14.430	1.00	47.69	B
7508	OH	TYR	B	1493	16.759	8.578	13.363	1.00	45.65	B
7509	C	TYR	B	1493	19.140	13.496	16.956	1.00	49.64	B
7510	O	TYR	B	1493	18.062	14.048	16.548	1.00	52.39	B
7511	OXT	TYR	B	1493	20.255	13.799	16.413	1.00	46.28	B
7512	O18	XYZ	C	1	-3.838	-4.342	38.231	1.00	82.39	C
7513	C17	XYZ	C	1	-3.375	-5.331	38.491	1.00	82.39	C
7514	C16	XYZ	C	1	-3.588	-6.515	37.603	1.00	82.39	C
7515	C15	XYZ	C	1	-2.651	-6.433	36.386	1.00	82.39	C
7516	C14	XYZ	C	1	-2.513	-7.808	35.714	1.00	82.39	C
7517	C13	XYZ	C	1	-1.231	-7.897	34.846	1.00	82.39	C
7518	C12	XYZ	C	1	-0.075	-8.432	35.683	1.00	82.39	C
7519	C11	XYZ	C	1	0.650	-7.591	36.482	1.00	82.39	C
7520	C8	XYZ	C	1	1.798	-8.108	37.369	1.00	82.39	C
7521	O9	XYZ	C	1	1.491	-9.351	38.094	1.00	82.39	C
7522	C10	XYZ	C	1	1.645	-10.598	37.336	1.00	82.39	C
7523	C6	XYZ	C	1	2.222	-7.079	38.393	1.00	82.39	C
7524	O7	XYZ	C	1	1.917	-5.646	37.881	1.00	82.39	C
7525	C4	XYZ	C	1	1.676	-7.359	39.857	1.00	82.39	C
7526	C5	XYZ	C	1	2.510	-6.519	40.866	1.00	82.39	C
7527	C3	XYZ	C	1	0.210	-6.909	40.120	1.00	82.39	C
7528	C2	XYZ	C	1	-0.963	-7.562	39.863	1.00	82.39	C
7529	C1	XYZ	C	1	-1.066	-8.931	39.244	1.00	82.39	C
7530	C20	XYZ	C	1	-2.312	-6.860	40.262	1.00	82.39	C
7531	C19	XYZ	C	1	-2.457	-5.395	39.707	1.00	82.39	C
7532	O	HOH	W	1	-22.823	3.020	18.627	1.00	65.23	W
7533	O	HOH	W	2	-8.627	8.401	44.702	1.00	63.79	W
7534	O	HOH	W	3	-19.265	21.432	27.751	1.00	75.34	W
7535	O	HOH	W	4	33.378	31.211	8.989	1.00	75.04	W
7536	O	HOH	W	5	-14.549	-31.394	24.843	1.00	60.50	W
7537	O	HOH	W	6	33.114	-11.026	13.023	1.00	59.44	W
7538	O	HOH	W	7	-33.460	-30.942	12.212	1.00	64.45	W
7539	O	HOH	W	8	22.793	-15.306	-2.398	1.00	57.16	W
7540	O	HOH	W	9	-30.598	25.384	28.884	1.00	67.50	W
7541	O	HOH	W	10	11.971	31.978	1.485	1.00	78.33	W
7542	O	HOH	W	11	14.437	4.260	40.537	1.00	84.53	W
7543	O	HOH	W	12	-0.602	40.561	5.615	1.00	54.70	W
7544	O	HOH	W	13	-37.458	25.807	14.873	1.00	80.19	W
7545	O	HOH	W	14	-12.522	-22.963	24.635	1.00	54.03	W
7546	O	HOH	W	15	-12.965	21.504	22.541	1.00	62.67	W
7547	O	HOH	W	16	-29.898	28.147	54.991	1.00	53.66	W

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7548  O   HOH W  17   -12.464  16.104  27.398  1.00 65.82     W
7549  O   HOH W  18    41.614  28.299  19.175  1.00 67.17     W
7550  O   HOH W  19    30.094   6.672  16.982  1.00 57.62     W
7551  O   HOH W  20    18.827  29.361  -1.024  1.00 94.90     W
7552  O   HOH W  21    17.291  30.937  -5.675  1.00 72.11     W
7553  O   HOH W  22    26.398 -20.845   2.236  1.00 76.75     W
7554  O   HOH W  23    17.735  47.299  22.787  1.00 67.73     W
7555  O   HOH W  24    15.126  -6.940  27.558  1.00 62.60     W
7556  O   HOH W  25   -18.630  24.444  58.518  1.00 67.49     W
7557  O   HOH W  26     4.167 -10.720   3.052  1.00 80.75     W
7558  O   HOH W  27   -26.145  -9.011  32.901  1.00 66.11     W
7559  O   HOH W  28   -27.515   8.571  37.231  1.00 77.41     W
7560  O   HOH W  29     7.394  -4.900   9.720  1.00 50.67     W
7561  O   HOH W  30   -21.185   3.572  47.583  1.00 56.13     W
7562  O   HOH W  31   -13.310  13.584  27.184  1.00 77.62     W
7563  O   HOH W  32    31.704   1.032  10.546  1.00 54.63      W
7564  O   HOH W  33   -16.045   2.583  46.242  1.00 81.79     W
7565  O   HOH W  34    -5.072  44.351  26.027  1.00 66.82     W
7566  O   HOH W  35   -25.935  32.174  42.499  1.00 66.94     W
7567  O   HOH W  36    -8.888   0.244  39.543  1.00 73.20     W
7568  O   HOH W  37   -36.958   0.231  13.776  1.00 74.47     W
7569  O   HOH W  38    37.355  37.679  10.419  1.00 97.11     W
7570  O   HOH W  39    27.522  13.270  11.803  1.00 91.10     W
7571  O   HOH W  40    32.761  -2.760  12.373  1.00 53.44     W
7572  O   HOH W  41   -33.563   3.380  33.650  1.00 75.63     W
7573  O   HOH W  42     8.406  10.941   7.956  1.00 59.61     W
7574  O   HOH W  43   -25.269  35.823  49.155  1.00 93.03     W
7575  O   HOH W  44    11.064  12.373  30.025  1.00 78.73     W
7576  O   HOH W  45    14.300   0.448   1.401  1.00 74.34     W
7577  O   HOH W  46    22.689  33.320   6.116  1.00 99.20     W
7578  O   HOH W  47    19.755  -9.006  -0.421  1.00 74.28     W
7579  O   HOH W  48   -15.215  30.874  30.724  1.00 90.34     W
7580  O   HOH W  49     2.226 -11.036  33.149  1.00 73.86     W
7581  O   HOH W  50   -30.305   4.027   8.547  1.00 66.08     W
7582  O   HOH W  51     8.083   9.384   4.015  1.00 87.70     W
7583  O   HOH W  52     9.847  19.520  25.157  1.00 68.60     W
7584  O   HOH W  53    -4.076   8.424  28.306  1.00 62.71     W
7585  O   HOH W  54   -13.137  36.123  37.081  1.00 79.64     W
7586  O   HOH W  55     2.591  45.059  28.074  1.00 97.38     W
7587  O   HOH W  56    32.996  11.321   4.805  1.00 51.94     W
7588  O   HOH W  57   -14.588  29.251  52.453  1.00 60.64     W
7589  O   HOH W  58   -10.962  24.049  31.004  1.00 83.64     W
7590  O   HOH W  59   -19.370  22.081  19.330  1.00 71.94     W
END
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All patents and publications referenced or mentioned herein are indicative of the levels of skill of those skilled in the art to which the invention pertains, and each such referenced patent or publication is hereby incorporated by reference to the same extent as if it had been incorporated by reference in its entirety individually or set forth herein in its entirety. Applicants reserve the right to physically incorporate into this specification any and all materials and information from any such cited patents or publications.

The specific methods and compositions described herein are representative of preferred embodiments and are exemplary and not intended as limitations on the scope of the invention. Other objects, aspects, and embodiments will occur to those skilled in the art upon consideration of this specification, and are encompassed within the spirit of the invention as defined by the scope of the claims. It will be readily apparent to one skilled in the art that varying substitutions and modifications may be made to the invention disclosed herein without departing from the scope and spirit of the invention. The invention illustratively described herein suitably may be practiced in the absence of any element or elements, or limitation or limitations, which is not specifically disclosed herein as essential. The methods and processes illustratively described herein suitably may be practiced in differing orders of steps, and that they are not necessarily restricted to the orders of steps indicated herein or in the claims. As used herein and in the appended claims, the singular forms "a," "an," and "the" include plural reference unless the context clearly dictates otherwise. Thus, for example, a reference to "a host cell" includes a plurality (for example, a culture or population) of such host cells, and so forth. Under no circumstances may the patent be interpreted to be limited to the specific examples or embodiments or methods specifically disclosed herein. Under no circumstances may the patent be interpreted to be limited by any statement made by any Examiner or any other official or employee of the Patent and Trademark Office unless such statement is specifically and without qualification or reservation expressly adopted in a responsive writing by Applicants.

The terms and expressions that have been employed are used as terms of description and not of limitation, and there is no intent in the use of such terms and

expressions to exclude any equivalent of the features shown and described or portions thereof, but it is recognized that various modifications are possible within the scope of the invention as claimed. Thus, it will be understood that although the present invention has been specifically disclosed by preferred embodiments and optional features, modification and variation of the concepts herein disclosed may be resorted to by those skilled in the art, and that such modifications and variations are considered to be within the scope of this invention as defined by the appended claims.

The invention has been described broadly and generically herein. Each of the narrower species and subgeneric groupings falling within the generic disclosure also form part of the invention. This includes the generic description of the invention with a proviso or negative limitation removing any subject matter from the genus, regardless of whether or not the excised material is specifically recited herein.

Other embodiments are within the following claims. In addition, where features or aspects of the invention are described in terms of Markush groups, those skilled in the art will recognize that the invention is also thereby described in terms of any individual member or subgroup of members of the Markush group.

WHAT IS CLAIMED:

1. A method of inhibiting fascin expression and/or activity, comprising administering an effective amount of a fascin inhibitor to a cell expressing fascin to thereby inhibit the fascin expression or activity in the cell.

2. The method of claim 1, wherein the fascin inhibitor comprises an inhibitory nucleic acid that binds specifically to a fascin RNA or DNA consisting of SEQ ID NO:2, 4, 6 or 8, a small molecule, a fascin polypeptide fragment, or an antibody that binds specifically to fascin.

3. The method of claim 2, wherein the inhibitory nucleic acid is an RNA or DNA consisting of any of SEQ ID NOs:13-62.

4. The method of claim 3, wherein the inhibitory nucleic acid is administered by administering an expression vector comprising an expression cassette that directs the expression of the inhibitory nucleic acid.

5. The method of claim 2, wherein the antibody blocks actin binding to a fascin actin-binding site or binds specifically to a fascin actin-binding site.

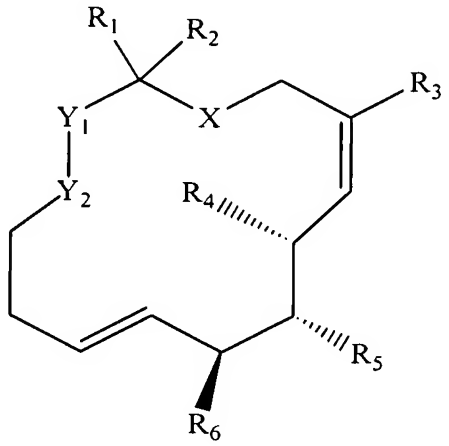
6. The method of claim 5, wherein the fascin actin-binding site comprises any of fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250.

7. The method of claim 6, wherein the fascin actin-binding site comprises any of fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473.

8. The method of claim 5, wherein the antibody blocks actin binding to one or both of fascin amino acids His392 and His474 when bound to fascin protein.

9. The method of claim 5, wherein the antibody binds to one or both of fascin amino acids His392 and His474 when bound to fascin protein.

10. The method of claim 1 or 2, wherein the fascin inhibitor is a compound of formula I:



wherein:

X is CH, N, NH or O;

R_1 is OH, CZ_3 or R_1 and R_2 together are –C=O, wherein Z is halo;

R_2 is OH, CZ_3 or R_1 and R_2 together are –C=O, wherein Z is halo;

R_3 is H or lower alkyl;

R_4 is H or lower alkyl;

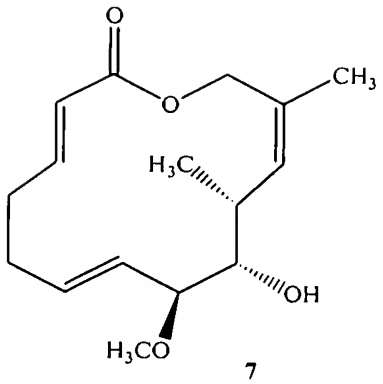
R_5 is OH;

R_6 is alkyloxy;

Y_1 and Y_2 are separately $–CH_2–$ or Y_1 and Y_2 together form –C=C–

or a pharmaceutically acceptable salt thereof.

11. The method of claim 10, wherein the compound is any one of the following compounds, or a combination thereof:



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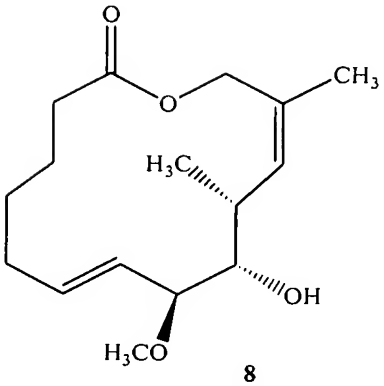

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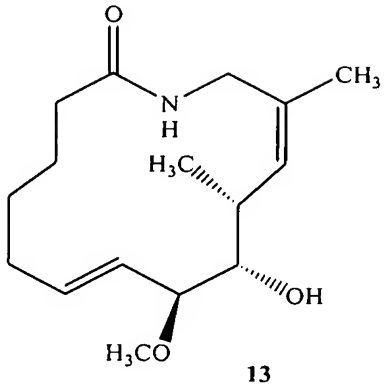

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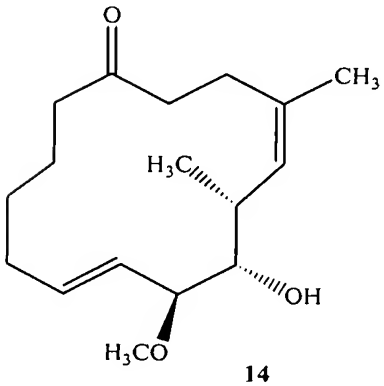

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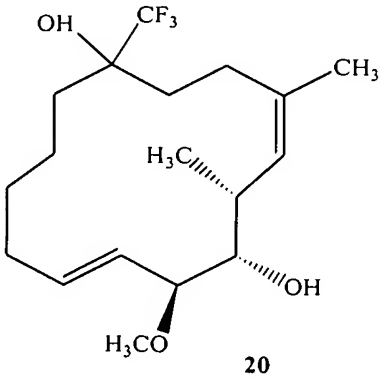

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12. The method of claim 2, wherein the fascin polypeptide fragment comprises fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250.

13. The method of claim 2, wherein the fascin polypeptide fragment comprises fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473.

14. The method of claim 12 or 13, wherein the fascin polypeptide fragment consists of fascin amino acids 259 through 493.

15. The fascin inhibitor of claim 2, wherein the fascin polypeptide fragment consists of SEQ ID NO:9, 10 and/or 12

16. The method of any of claims 1-15, wherein the cell is in an animal.

17. The method of claim 16, wherein the animal is a human.

18. The method of claim 17, wherein the human suffers from a disease or condition.

19. The method of claim 18, wherein the disease or condition is a metastatic cancer, a neuronal disorder, neuronal degeneration, an inflammatory condition, a viral infection, a bacterial infection, lymphoid hyperplasia, Hodgkin's disease or ischemia-related tissue damage.

20. The method of claim 19, wherein the cancer is a carcinoma, lymphoma, sarcoma, melanoma, astrocytoma, mesothelioma cells, ovarian carcinoma, colon carcinoma, pancreatic carcinoma, esophageal carcinoma, stomach carcinoma, lung carcinoma, urinary carcinoma, bladder carcinoma, breast cancer, gastric cancer, leukemia, lung cancer, colon cancer, central nervous system cancer, melanoma, ovarian cancer, renal cancer or prostate cancer.

21. A method of identifying an inhibitor of fascin, comprising:

a) contacting at least one protein or peptide having a fascin sequence with at least one test agent for a sufficient time to allow the components to interact; and

b) determining whether binding between the at least one protein or peptide having a fascin sequence and the test agent has occurred,

wherein binding between the at least one protein or peptide having a fascin sequence and test agent is indicative that the test agent is an inhibitor of cancer metastasis.

22. The method of claim 21, wherein the test agent blocks actin binding to a fascin actin-binding site or binds to a fascin actin-binding site.

23. The method of claim 21 or 22, wherein the fascin actin-binding site comprises fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250.

24. The method of claim 21 or 22, wherein the fascin actin-binding site comprises fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473.

25. The method of any of claims 21, 22 or 24, wherein the test agent blocks actin binding to one or both of fascin amino acids His392 and His474 when bound to fascin protein.

26. The method of any of claims 21, 22 or 24, wherein the test agent binds to one or both of fascin amino acids His392 and His474 when bound to fascin protein.

27. The method of any of claims 21-26, further comprising determining the binding constant of the test agent for fascin.

28. The method of any of claims 21-27, further comprising determining whether the test agent inhibits fascin-mediated actin bundle formation.

29. The method of claim 28, wherein the actin is F-actin.

30. A method for identifying an inhibitor of fascin, comprising:

a) generating a three-dimensional structural image of a fascin binding site from fascin atomic coordinates for fascin amino acids Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250, according to Table 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms; and

b) designing or selecting a potential inhibitor to reside within the fascin binding site to thereby identify an inhibitor of fascin.

31. A method for identifying an inhibitor of fascin, comprising:

a) generating a three-dimensional structural image of a fascin binding site from fascin atomic coordinates for fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473 according to Table 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms; and

b) designing or selecting a potential inhibitor to reside within the fascin binding site to thereby identify an inhibitor of fascin.

32. The method of claim 30 or 31, further comprising synthesizing or obtaining the potential inhibitor, contacting the potential inhibitor with fascin, and ascertaining whether the potential inhibitor binds to fascin.

33. The method of any of claims 30-32, wherein the potential inhibitor is no larger than about eight (8) angstroms by about ten (10) angstroms by about ten (10) angstroms.

34. The method of any of claims 30-33, wherein the method is performed using a computer system comprising the fascin atomic coordinates as a data set.

35. The method of any of claims 21-34, wherein the inhibitor of fascin is an inhibitor of metastatic cancer.

36. A machine readable storage medium, comprising fascin atomic coordinates of Table 2.

37. The machine readable storage medium of claim 36, comprising fascin atomic coordinates for fascin amino acids Thr326, Ser328, Ser329, Lys 330 , Asn331, Ser333, Arg276,Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250, according to Table 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms.

38. The machine readable storage medium of claim 36, comprising fascin atomic coordinates for fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473 according to Table 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 angstroms.

39. A fascin inhibitor comprising an inhibitory nucleic acid that binds specifically to a fascin RNA or DNA consisting of SEQ ID NO:2, 4, 6 or 8, a small molecule, a fascin polypeptide fragment, or an antibody that binds specifically to fascin.

40. The fascin inhibitor of claim 39, wherein the inhibitory nucleic acid is an RNA or DNA consisting of any of SEQ ID NOs:13-62.

41. The fascin inhibitor of claim 39 or 40, wherein the inhibitory nucleic acid is expressed in an expression vector comprising an expression cassette that directs the expression of a fascin inhibitory nucleic acid.

42. The fascin inhibitor of claim 39, wherein the antibody binds specifically to a fascin actin-binding site, or blocks actin-binding to a fascin actin-binding site, wherein the actin-binding site comprises fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250.

43. The fascin inhibitor of claim 42, wherein the antibody binds specifically to a fascin actin-binding site, or blocks actin-binding to a fascin actin-binding site, wherein the actin-binding site comprises fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473.

44. The fascin inhibitor of claim 39 or 43, wherein the antibody was generated using a polypeptide with a sequence that includes fascin amino acids 259 through 493.

45. The fascin inhibitor of claim 39 or 43, wherein the antibody was generated using a polypeptide with SEQ ID NO:9, 10 and/or 12.

46. The fascin inhibitor of claim 39, wherein the fascin polypeptide fragment comprises fascin amino acids Thr326, Ser328, Ser329, Lys 330, Asn331, Ser333, Arg276, Gln 277, Met279, Asp286, Glu287, Gln291, Thr320, Thr318, Lys313, Thr311, Gln362, Asn360, Lys359, Asp168, Pro159, Arg151, Lys150, Arg149, Arg197, Arg201, Glu207, Glu227, Ser237, Pro236, Lys241, Lys247, and Lys250.

47. The fascin inhibitor of claim 39, wherein the fascin polypeptide fragment comprises fascin amino acids His392, Glu391, Ala488, Lys471, His474 and Asp473.

48. The fascin inhibitor of claim 39 or 47, wherein the fascin polypeptide fragment consists of fascin amino acids 259 through 493.

49. The fascin inhibitor of claim 39 or 48, wherein the fascin polypeptide fragment consists of SEQ ID NO:9, 10 and/or 12

50. A method of treating or inhibiting metastatic cancer in a patient, comprising administering to the patient, the fascin inhibitor of any of claims 39-49.

51. Use of a fascin inhibitor of any of claims 39-49 in the manufacture of a medicament.

52. The use of claim 51, wherein the medicament is for the treatment of metastatic cancer, a neuronal disorder, neuronal degeneration, an inflammatory condition, a viral infection, a bacterial infection, lymphoid hyperplasia, Hodgkin's disease or ischemia-related tissue damage.

53. The use of claim 51, wherein the medicament is for the treatment or inhibition of metastatic cancer in a mammal.

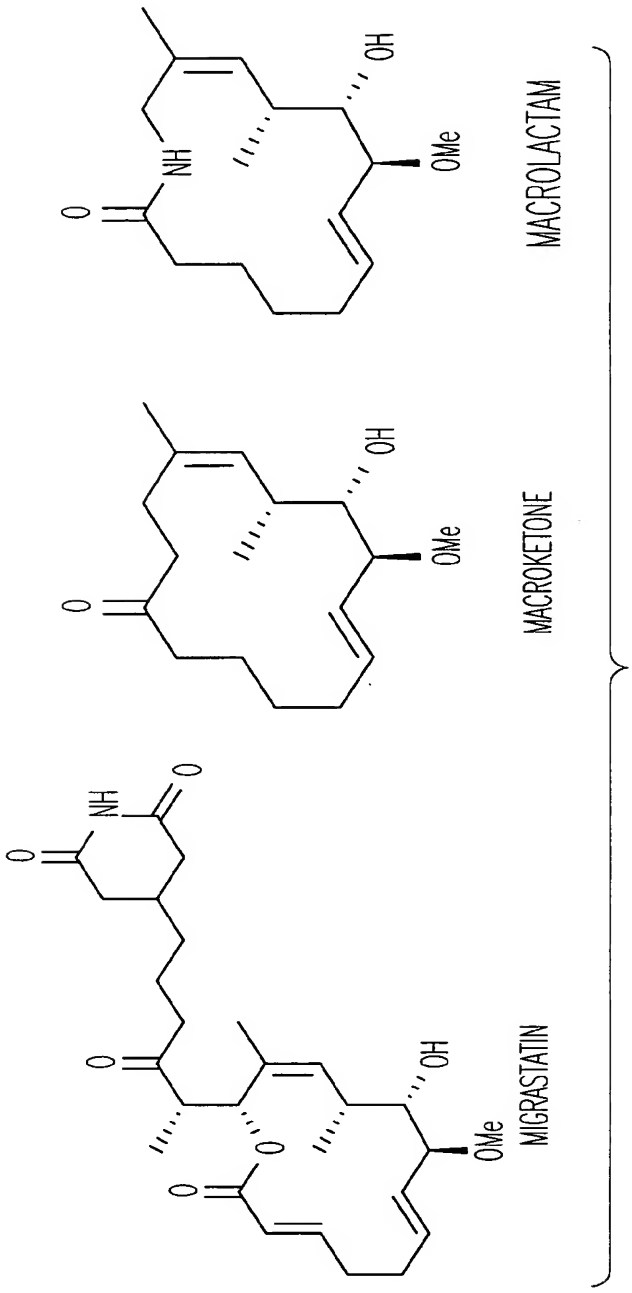

MIGRASTATIN
MACROKETONE
MACROLACTAM
OMe
OH
NH
O

Fig. 1A

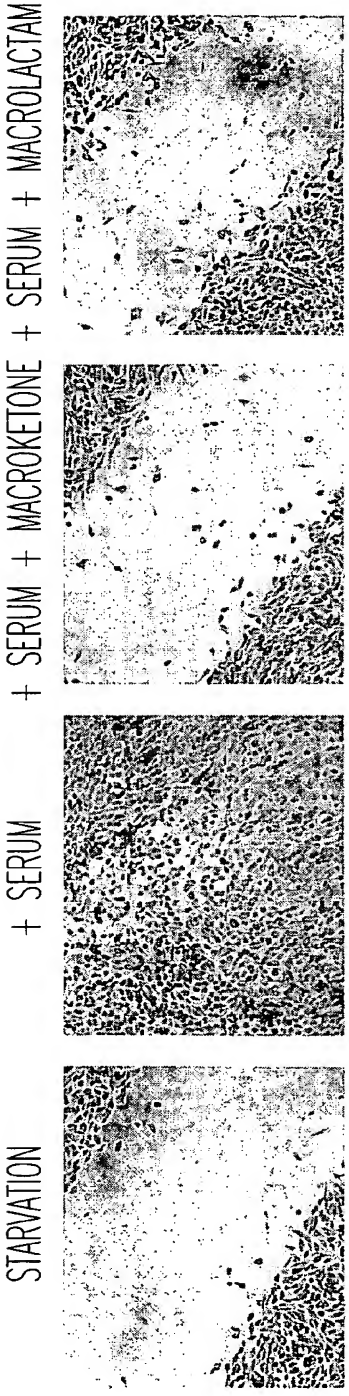

STARVATION
+ SERUM
+ SERUM + MACROKETONE
+ SERUM + MACROLACTAM

Fig. 1B

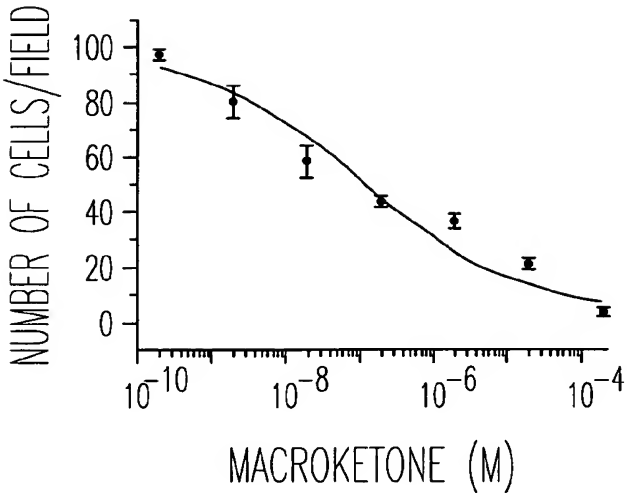

NUMBER OF CELLS/FIELD
100
80
60
40
20
0
10^{-10}
10^{-8}
10^{-6}
10^{-4}
MACROKETONE (M)

Fig. 1C

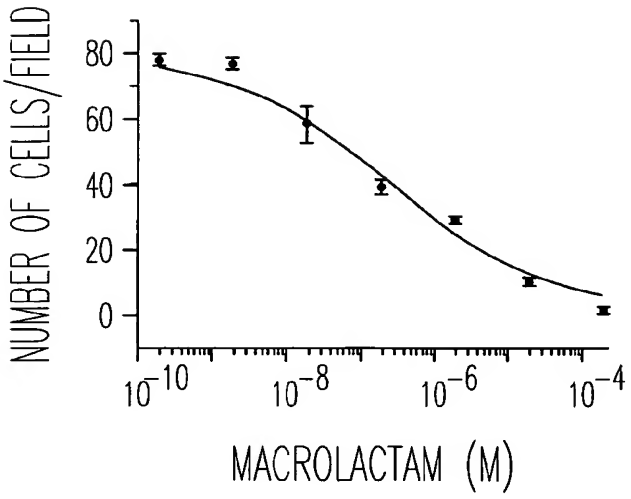

NUMBER OF CELLS/FIELD
80
60
40
20
0
10^{-10}
10^{-8}
10^{-6}
10^{-4}
MACROLACTAM (M)

Fig. 1D

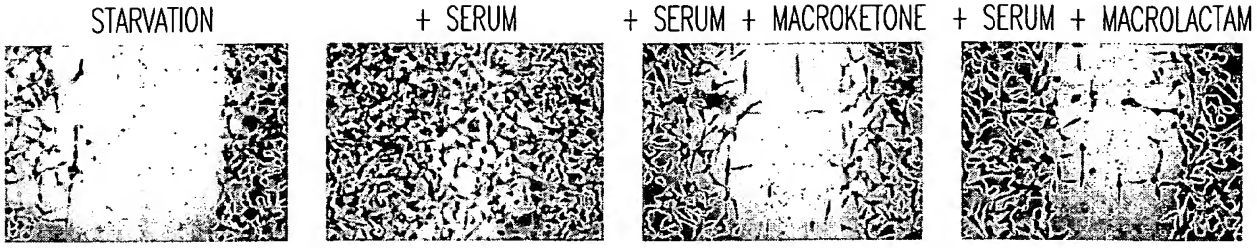


Fig. 2A

METASTATIC TUMOR CELLS	IC_{50} (μM)	
	MACROKETONE	MACROLACTAM
HUMAN BREAST TUMOR MDA-MB 231 CELLS	0.35	2.7
HUMAN COLON TUMOR LOVO CELLS	0.023	0.174
HUMAN PROSTATE TUMOR PC-3 CELLS	0.17	1.285

Fig. 2B

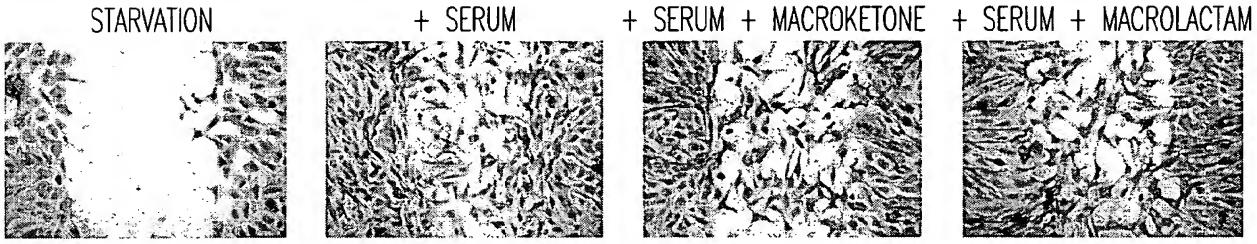


Fig. 2C

NORMAL CELLS	IC_{50} (μM)	
	MACROKETONE	MACROLACTAM
MOUSE MEF CELLS	>200	>200
HUMAN MAMMARY GLAND EPITHETICAL CELLS	137	>200
MOUSE LEUKOCYTES	>200	>200

Fig. 2D

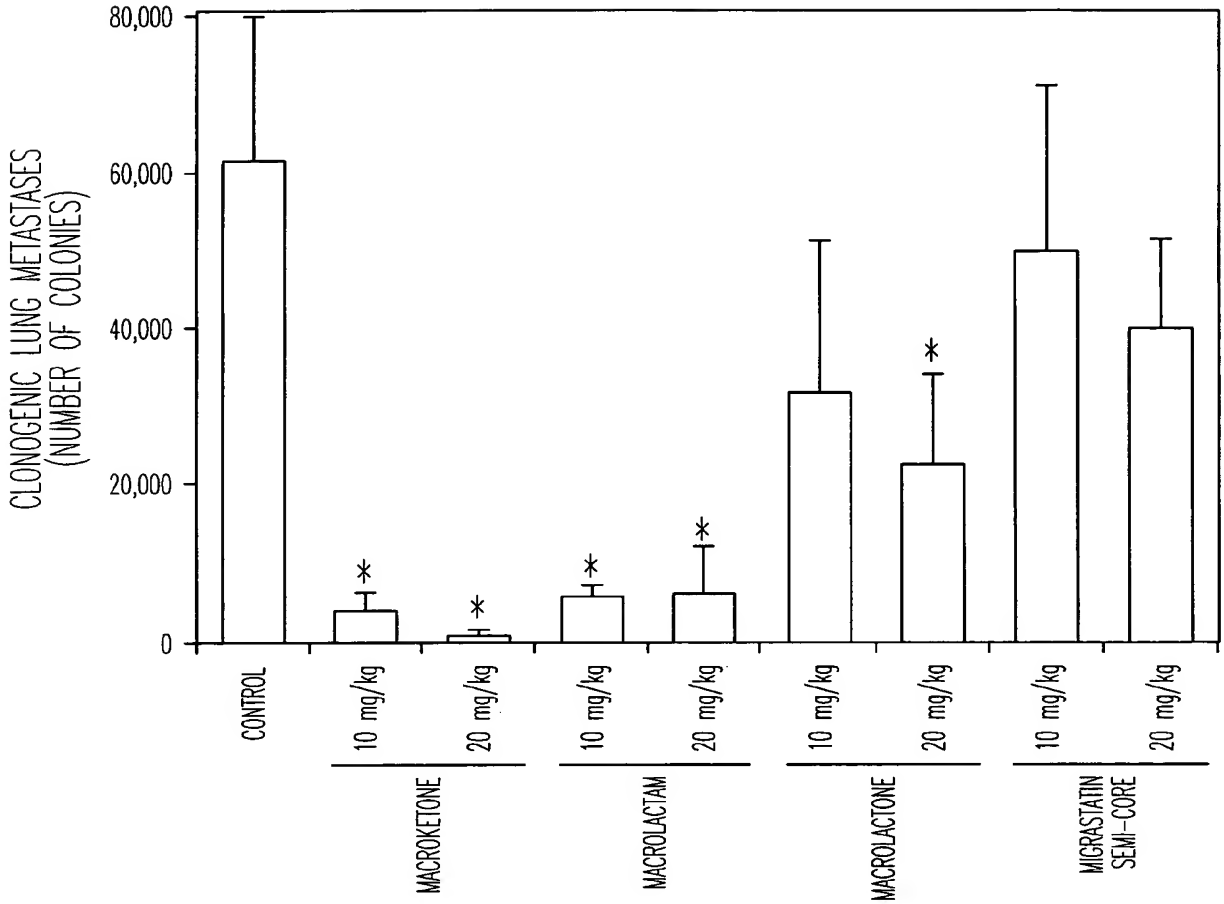

CLONOGENIC LUNG METASTASES (NUMBER OF COLONIES)
80,000
60,000
40,000
20,000
0
CONTROL
10 mg/kg
20 mg/kg
10 mg/kg
20 mg/kg
10 mg/kg
20 mg/kg
10 mg/kg
20 mg/kg
MACROKETONE
MACROLACTAM
MACROLACTONE
MIGRASTATIN SEMI-CORE

Fig. 3A

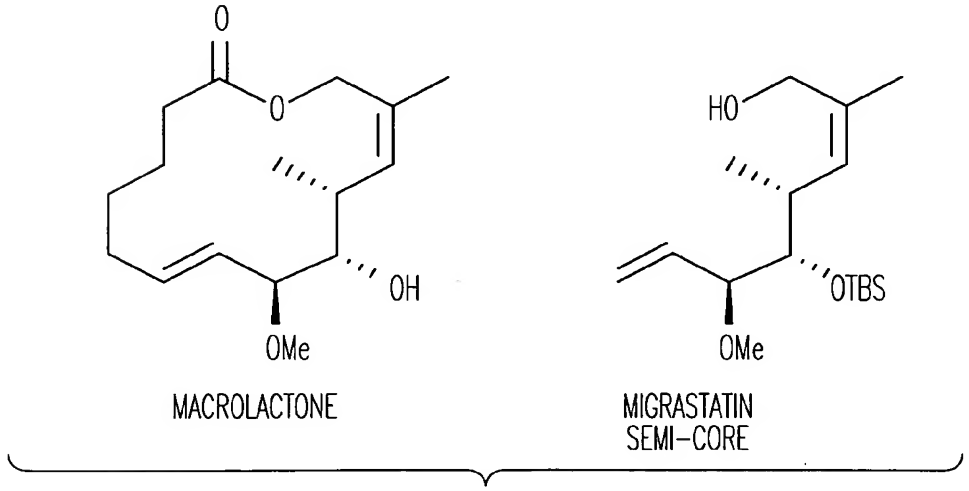

O
O
OH
OMe
HO
OTBS
OMe
MACROLACTONE
MIGRASTATIN SEMI-CORE

Fig. 3B

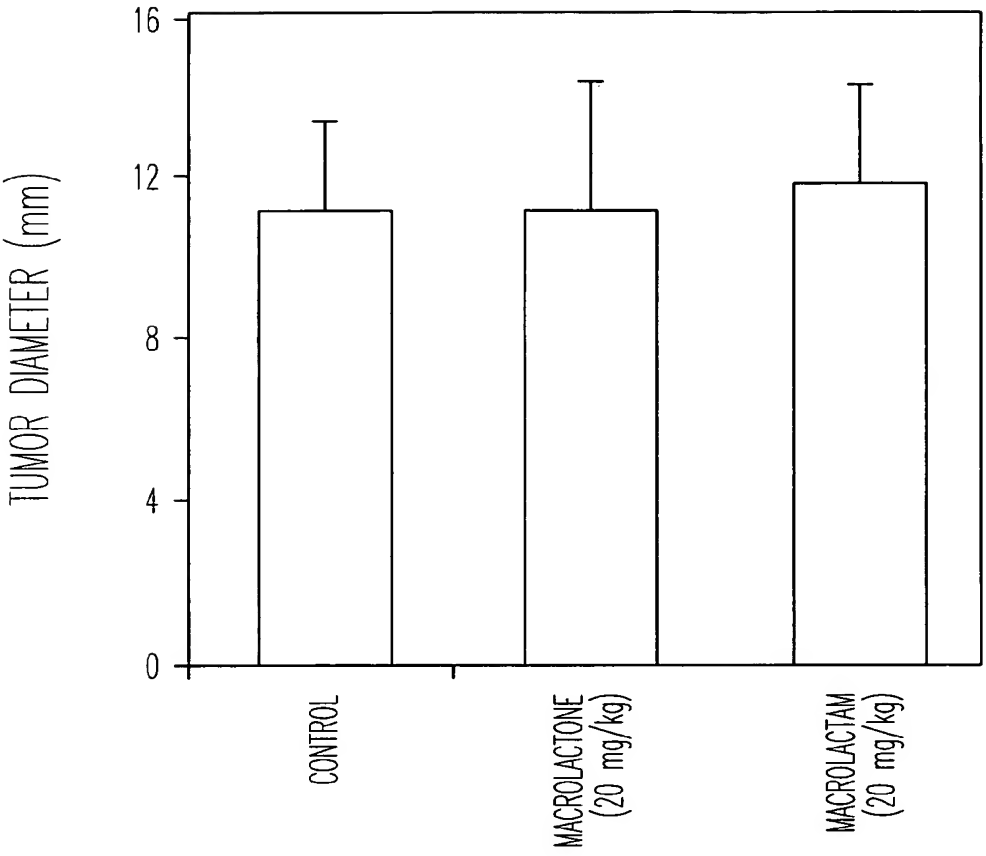
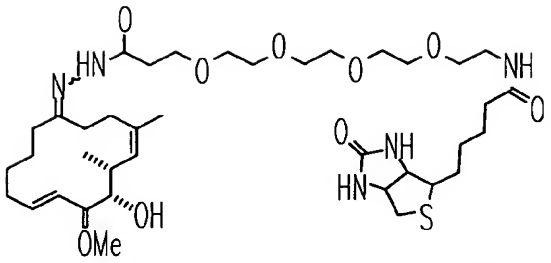

TUMOR DIAMETER (mm)
16
12
8
4
0
CONTROL
MACROLACTONE (20 mg/kg)
MACROLACTAM (20 mg/kg)

Fig. 3C



BIOTIN–CONJUGATED MACROKETONE

Fig. 4A

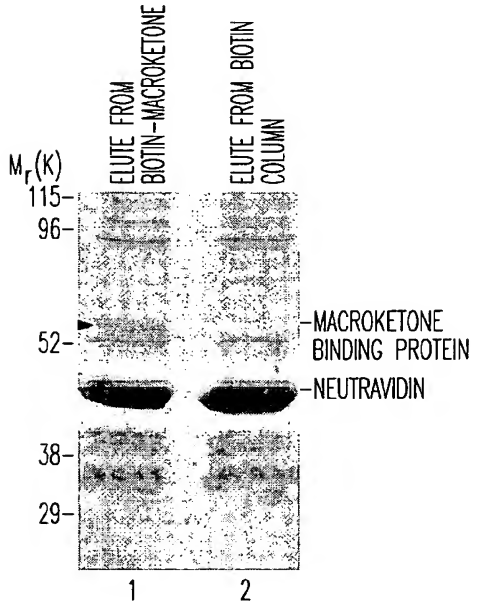


Fig. 4B

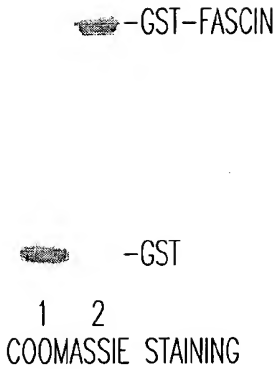


Fig. 5A

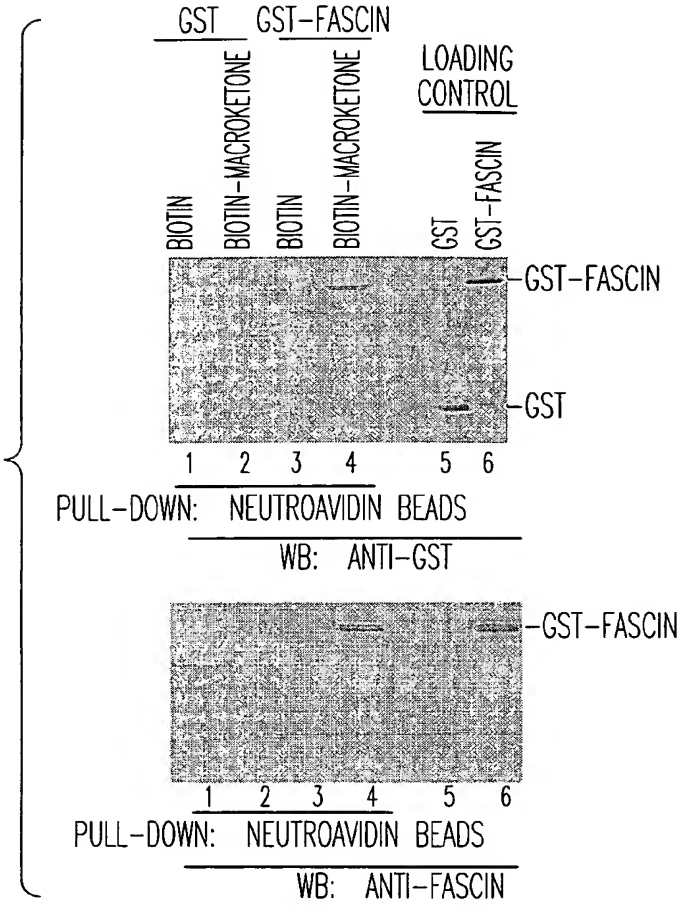


Fig. 5B

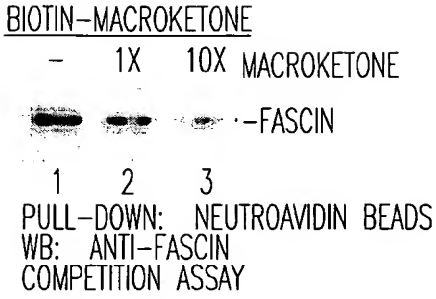


Fig. 5C

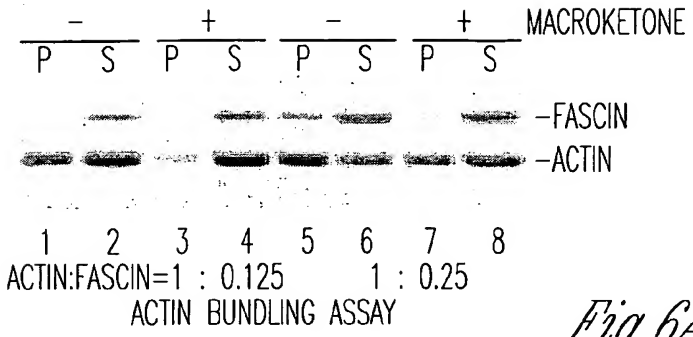


Fig. 6A

Fig. 6B

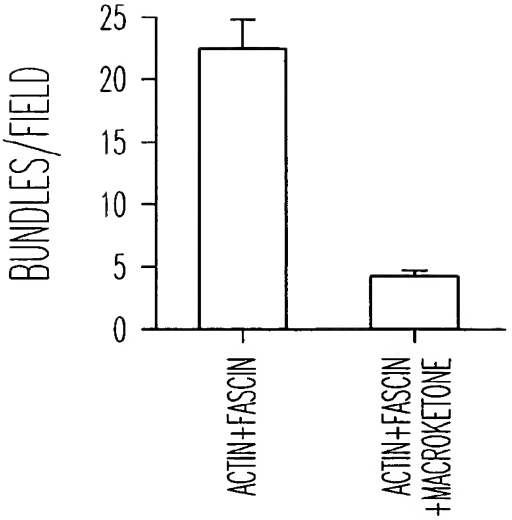


Fig. 6C

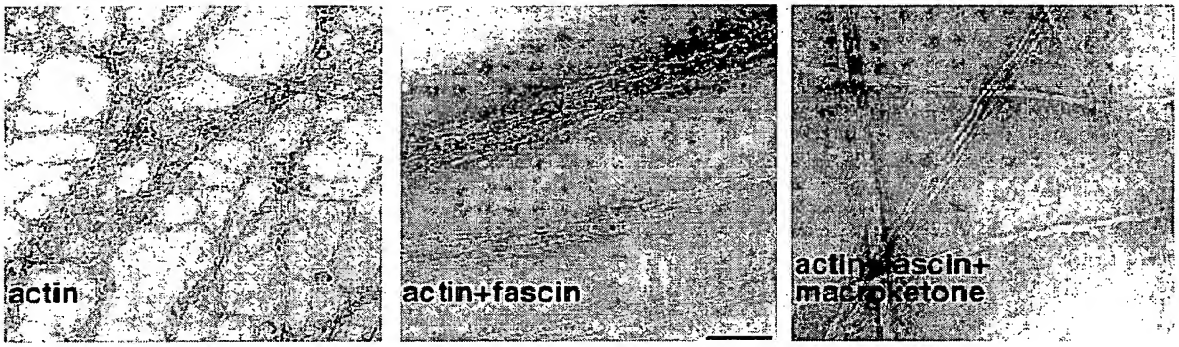
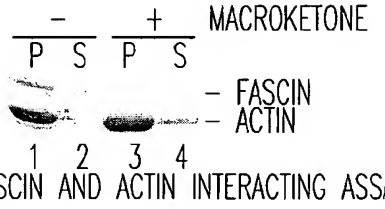


Fig. 6D



FASCIN AND ACTIN INTERACTING ASSAY

Fig. 6E

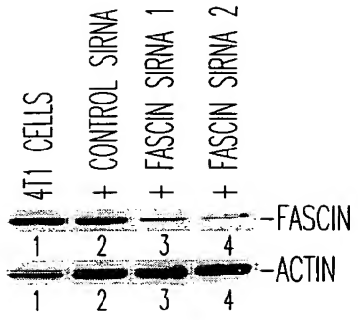


Fig. 7A

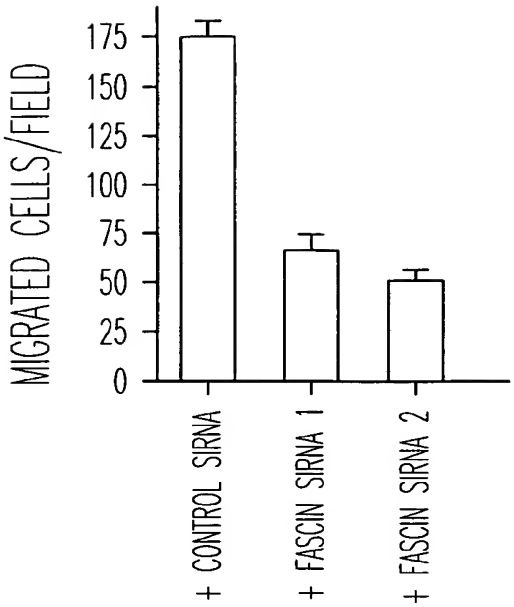
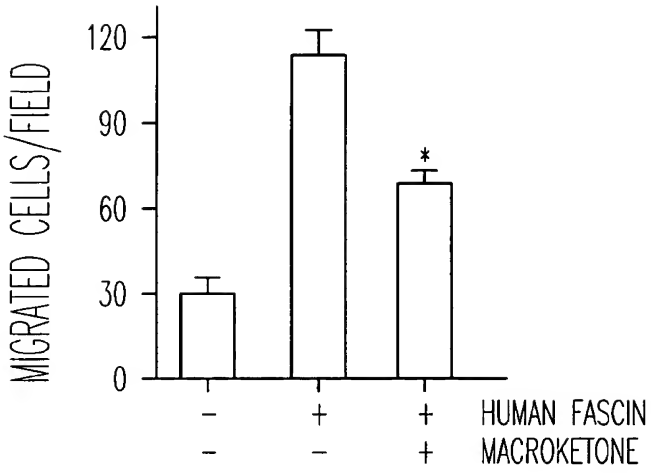


Fig. 7B



FASCIN SIRNA 2-TREATED 4T1 CELLS

Fig. 7C

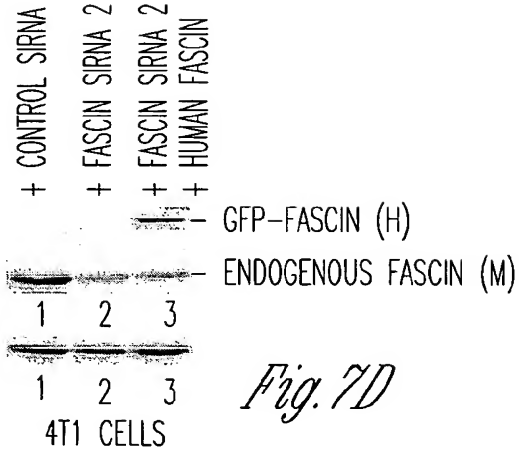


Fig. 7D

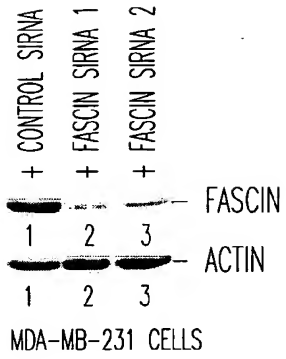


Fig. 7E

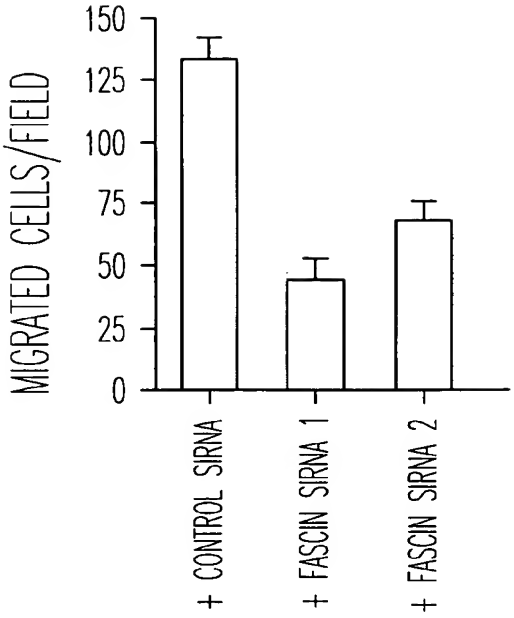


Fig. 7F

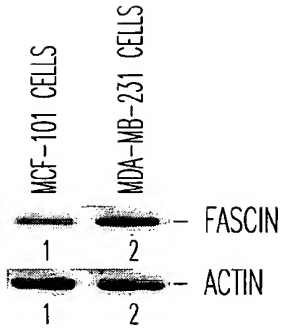


Fig. 7G

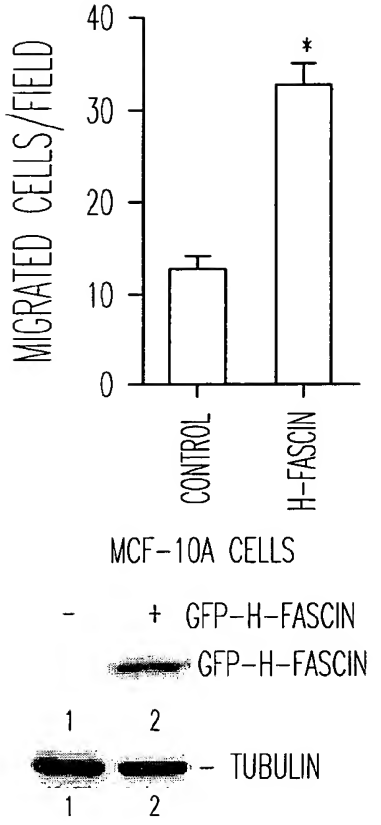

MIGRATED CELLS/FIELD
40
30
20
10
0
*
CONTROL
H-FASCIN
MCF-10A CELLS
- + GFP-H-FASCIN
GFP-H-FASCIN
1 2
TUBULIN
1 2

Fig. 7H

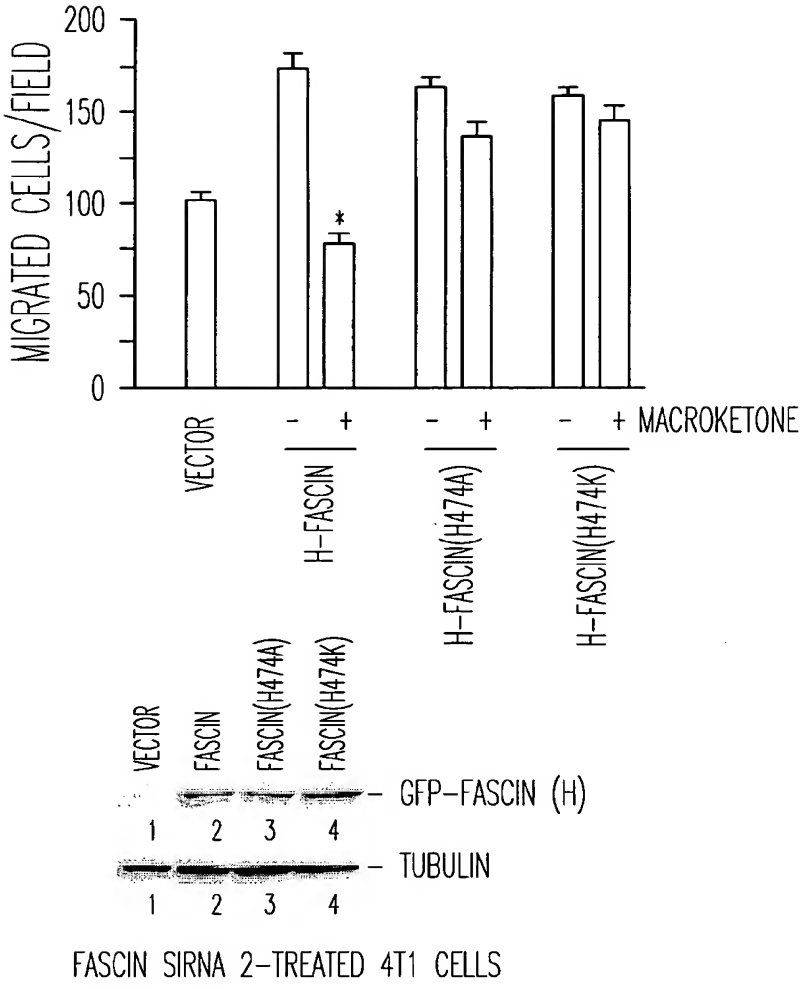

MIGRATED CELLS/FIELD
200
150
100
50
0
*
VECTOR
- + H-FASCIN
- + H-FASCIN(H474A)
- + H-FASCIN(H474K)
MACROKETONE
VECTOR
FASCIN
FASCIN(H474A)
FASCIN(H474K)
GFP-FASCIN (H)
1 2 3 4
TUBULIN
1 2 3 4
FASCIN SIRNA 2-TREATED 4T1 CELLS

Fig. 7I

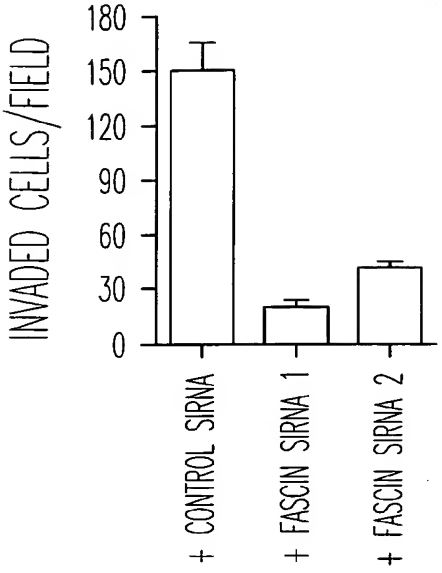


Fig. 8A

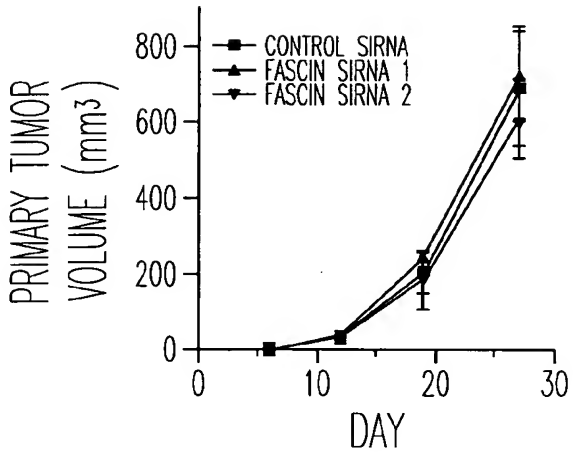


Fig. 8B

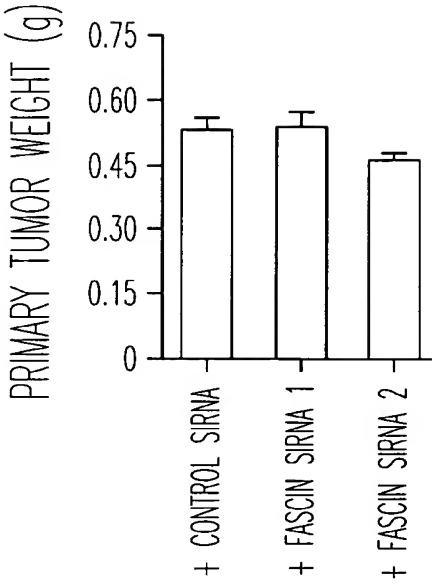


Fig. 8C

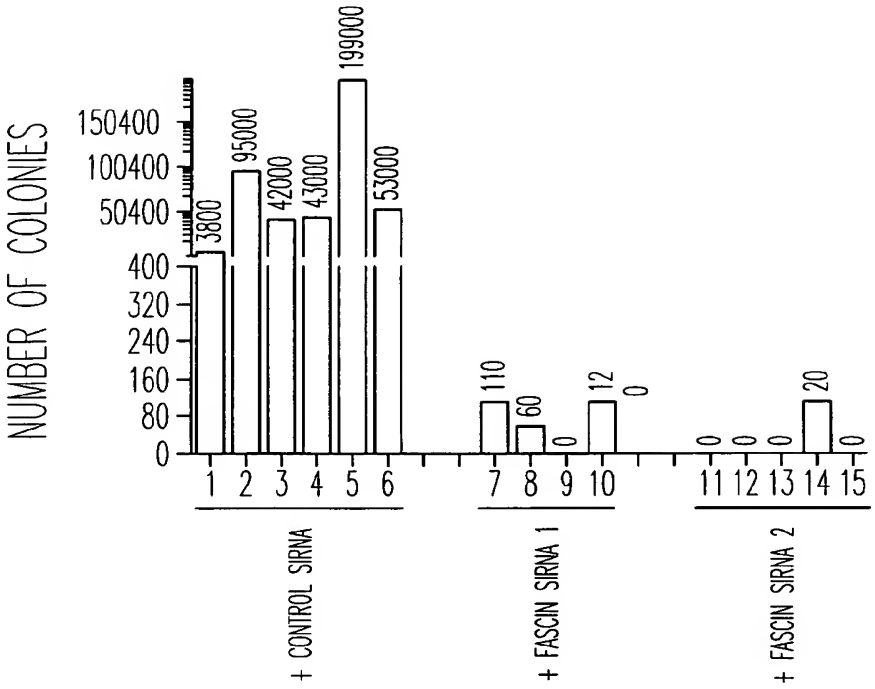

NUMBER OF COLONIES
150400
100400
50400
400
320
240
160
80
0
3800
95000
42000
43000
199000
53000
110
60
0
12
0
0
0
0
20
0
1 2 3 4 5 6
7 8 9 10
11 12 13 14 15
+ CONTROL SIRNA
+ FASCIN SIRNA 1
+ FASCIN SIRNA 2

Fig. 8D

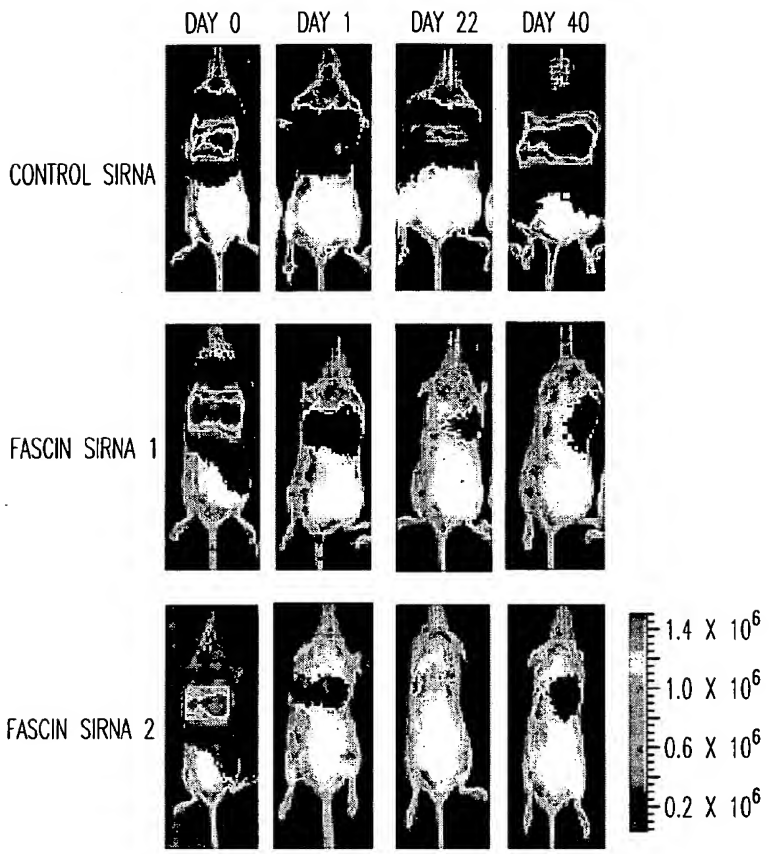

DAY 0
DAY 1
DAY 22
DAY 40
CONTROL SIRNA
FASCIN SIRNA 1
FASCIN SIRNA 2
1.4 X 10^6
1.0 X 10^6
0.6 X 10^6
0.2 X 10^6

Fig. 8E

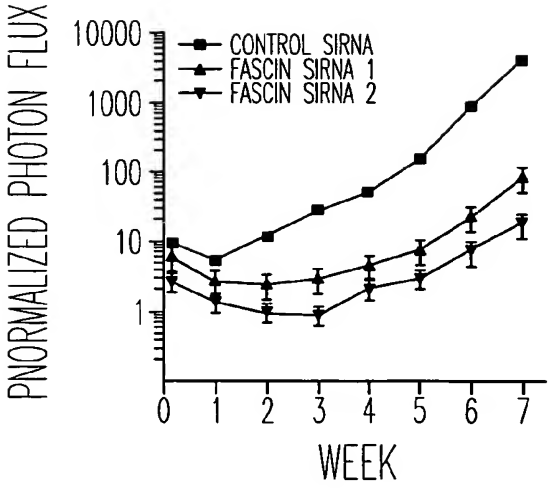

PNORMALIZED PHOTON FLUX
10000
1000
100
10
1
CONTROL SIRNA
FASCIN SIRNA 1
FASCIN SIRNA 2
0
1
2
3
4
5
6
7
WEEK

Fig. 8F

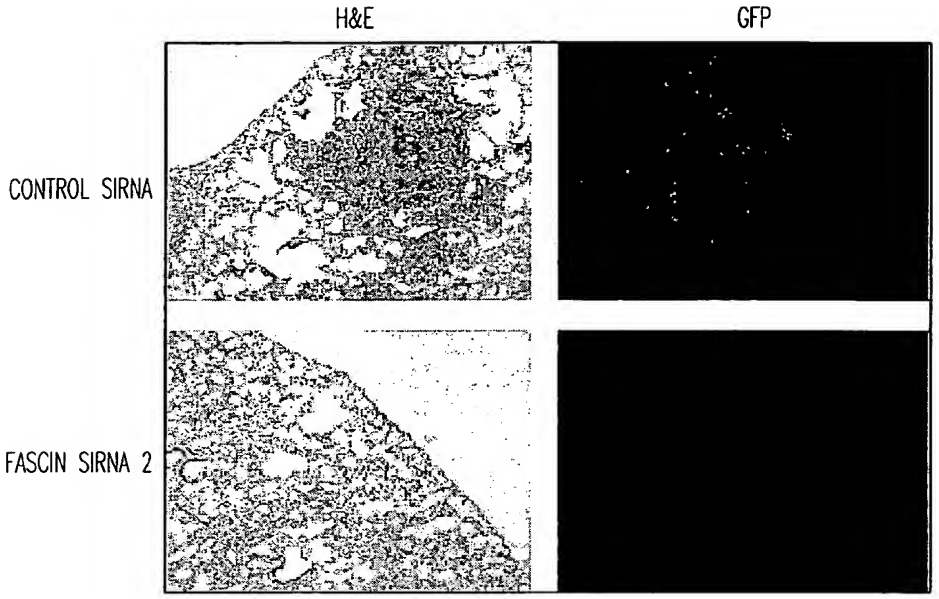

H&E
GFP
CONTROL SIRNA
FASCIN SIRNA 2

Fig. 8G

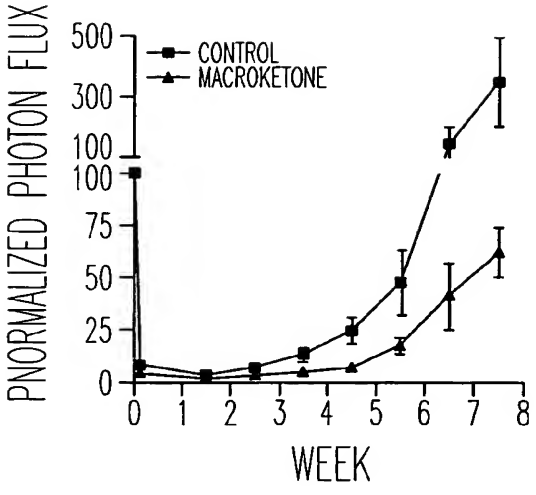

PNORMALIZED PHOTON FLUX
500
300
100
100
75
50
25
0
CONTROL
MACROKETONE
0 1 2 3 4 5 6 7 8
WEEK

Fig. 8H

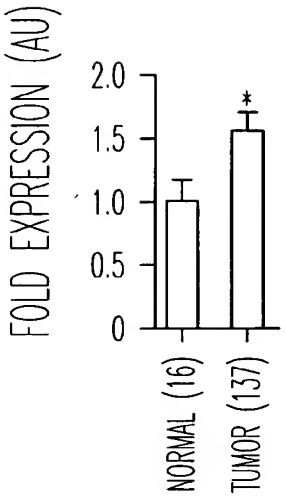


Fig. 9A

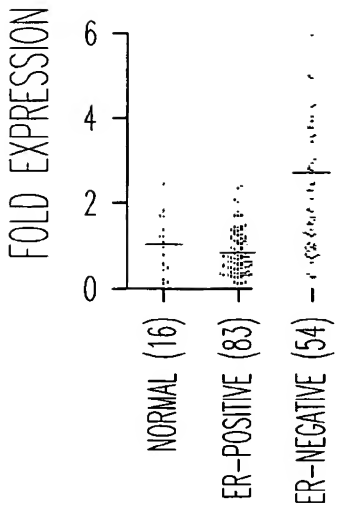


Fig. 9B

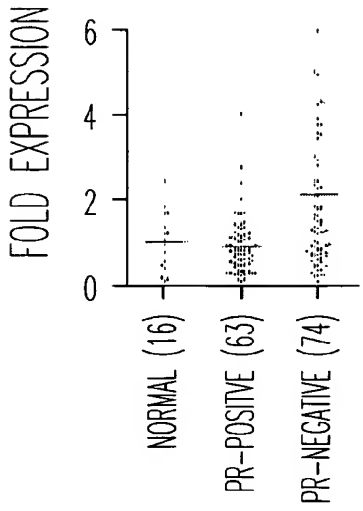


Fig. 9C

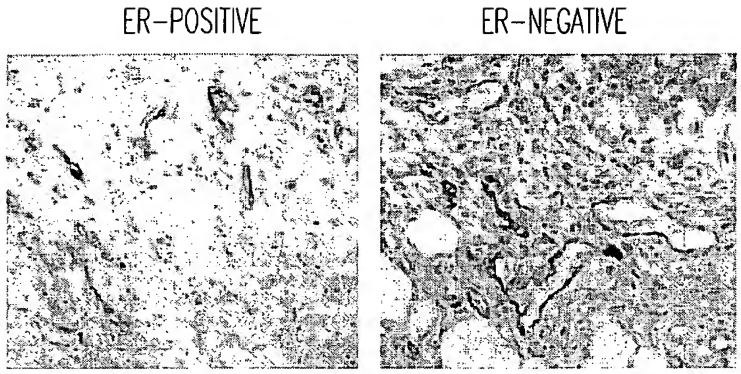


Fig. 9D

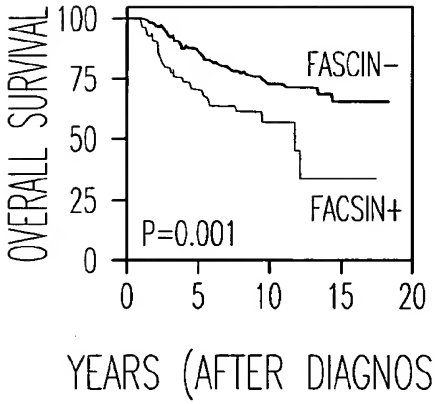


Fig. 9E

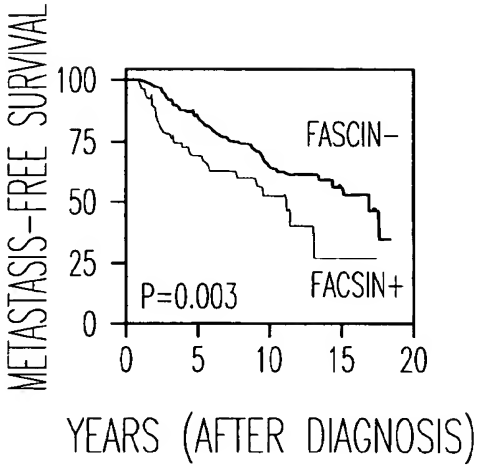


Fig. 9F

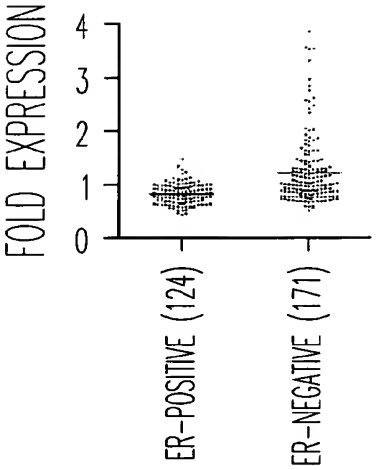

FOLD EXPRESSION
4
3
2
1
0
ER-POSITIVE (124)
ER-NEGATIVE (171)

Fig. 9G

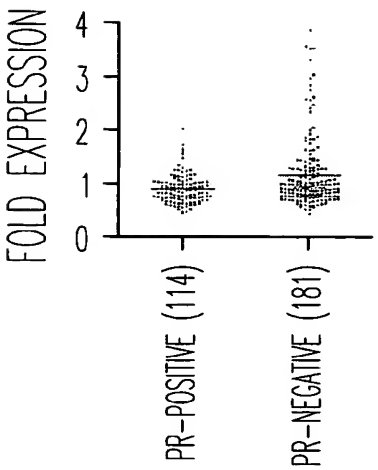

FOLD EXPRESSION
4
3
2
1
0
PR-POSITIVE (114)
PR-NEGATIVE (181)

Fig. 9H

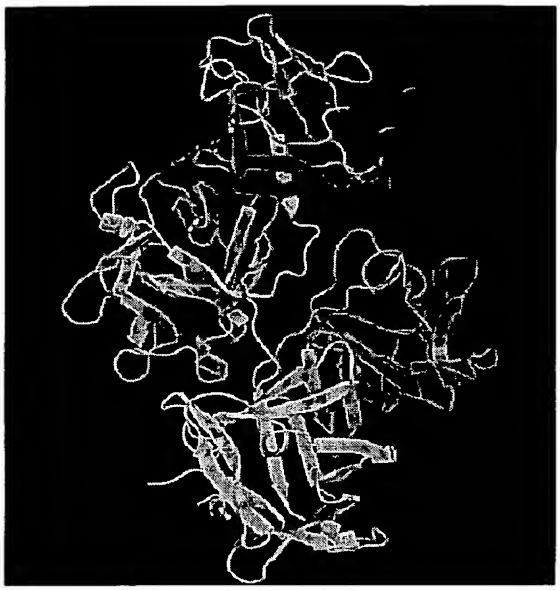


Fig. 10A

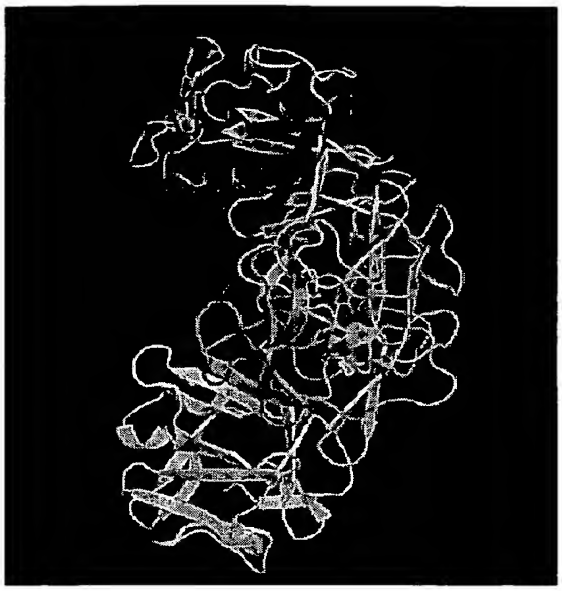


Fig. 10B

Fig. 10C

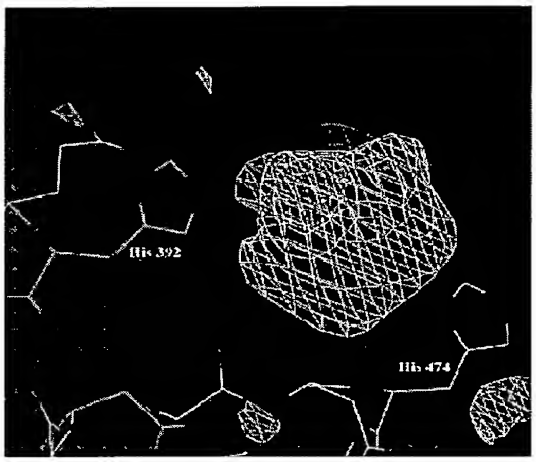


Fig. 11A

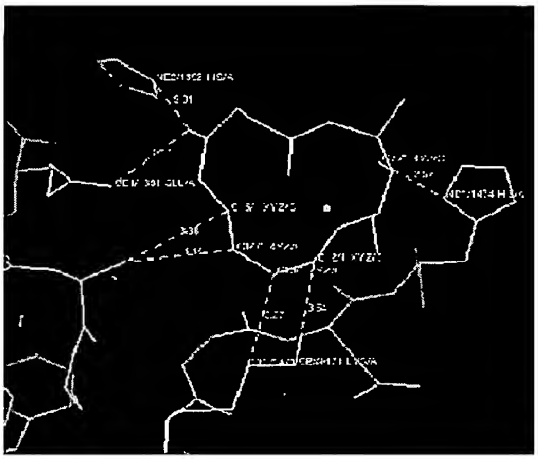


Fig. 11B

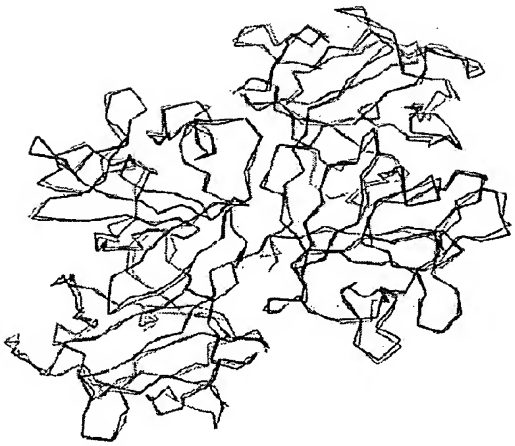


Fig. 11C

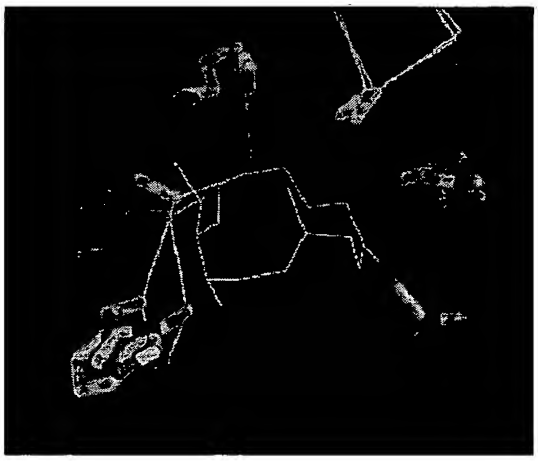


Fig. 11D

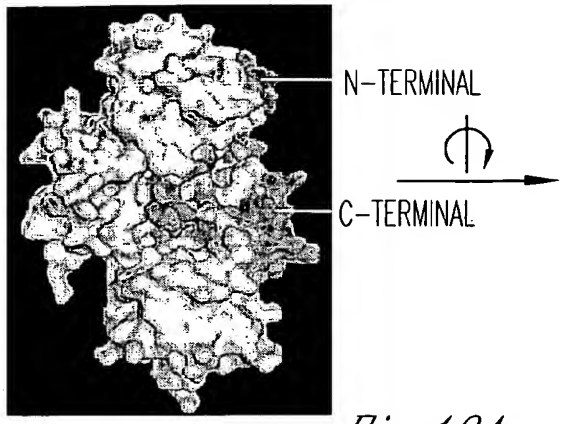


Fig. 12A

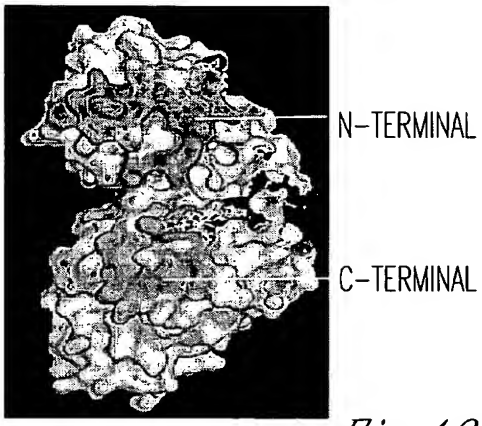


Fig. 12B

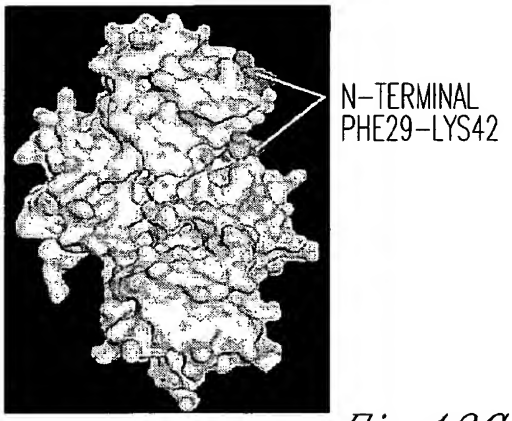


Fig. 12C

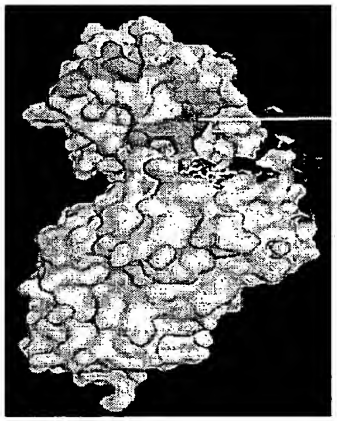


Fig. 12D

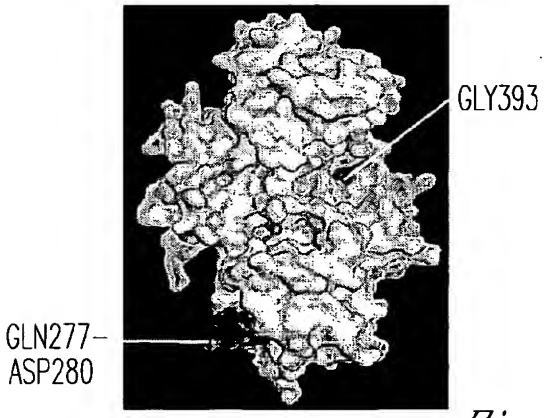


Fig. 12E

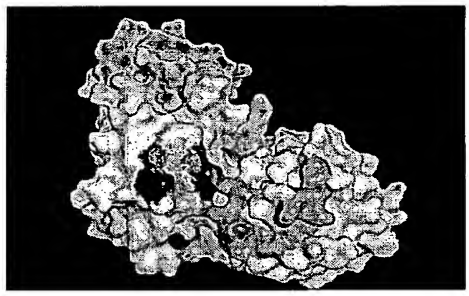


Fig. 13A

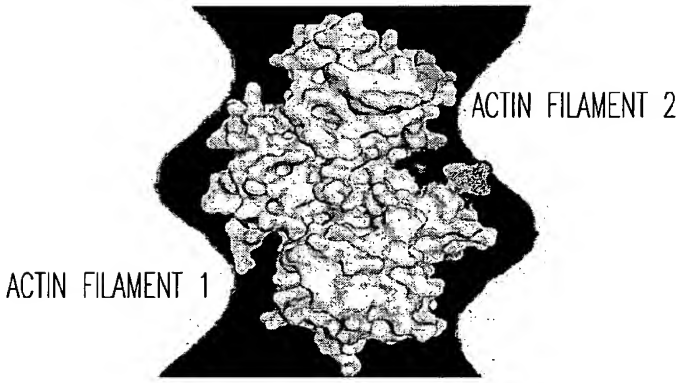


Fig. 13B

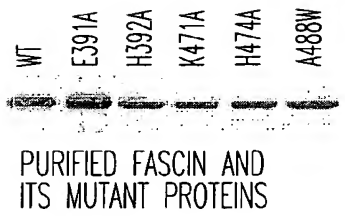


Fig. 14A

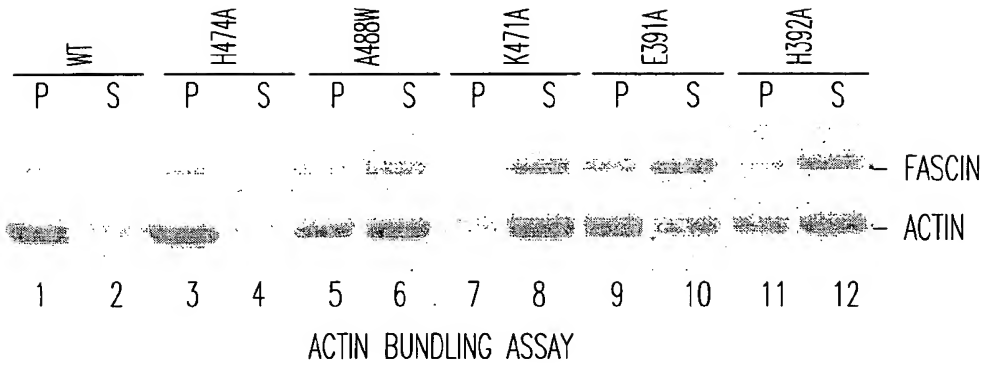


Fig. 14B

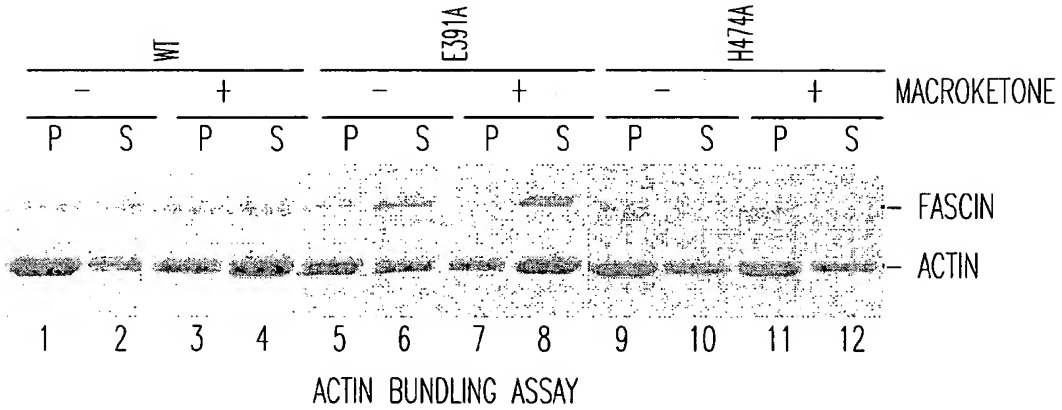


Fig. 14C

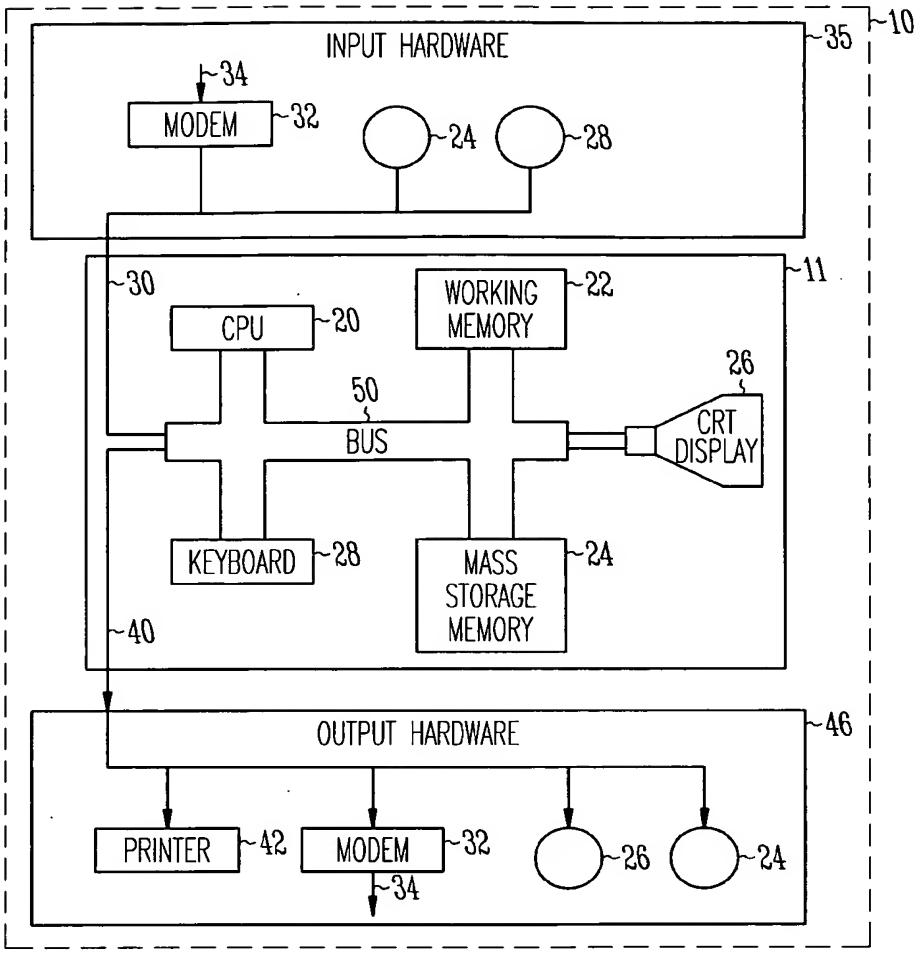


Fig. 15

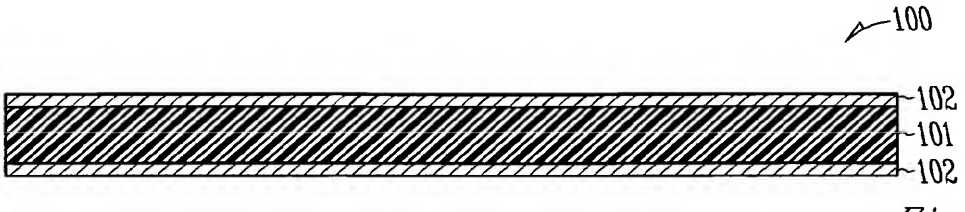


Fig. 16

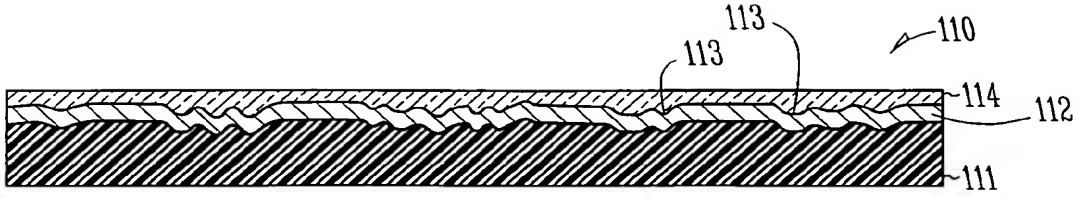


Fig. 17